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NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 FEB 25 CA/CAPLUS - Russian Agency for Patents and Trademarks
(ROSPATENT) added to list of core patent offices covered
NEWS 4 FEB 28 PATDPAFULL - New display fields provide for legal status
data from INPADOC
```

NEWS 5 FEB 28 BABS - Current-awareness alerts (SDIs) available

NEWS 6 FEB 28 MEDLINE/LMEDLINE reloaded

NEWS 7 MAR 02 GBFULL: New full-text patent database on STN

NEWS 8 MAR 03 REGISTRY/ZREGISTRY - Sequence annotations enhanced

NEWS 9 MAR 03 MEDLINE file segment of TOXCENTER reloaded

NEWS 10 MAR 22 KOREAPAT now updated monthly; patent information enhanced

NEWS 11 MAR 22 Original IDE display format returns to REGISTRY/ZREGISTRY

NEWS 12 MAR 22 PATDPASPC - New patent database available

NEWS 13 MAR 22 REGISTRY/ZREGISTRY enhanced with experimental property tags

NEWS  $14\ \text{APR}\ 04$  EPFULL enhanced with additional patent information and new fields

NEWS 15 APR 04 EMBASE - Database reloaded and enhanced

NEWS 16 APR 18 New CAS Information Use Policies available online

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
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NEWS WWW CAS World Wide Web Site (general information)

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=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0 DICTIONARY FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0

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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\10706448.str

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1 2 3 4 5 6 16 17 18 19 20 21 25 26 27 28 29 30 chain bonds : 1-7 1-32 2-22 2-33 7-8 7-15 8-9 8-10 10-11 11-12 11-14 12-13 12-17 21-35 22-23 22-31 23-24 23-29 26-34 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 25-26 25-30 26-27 27-28 28-29 29-30 exact/norm bonds : 1-7 2-22 7-8 8-9 11-12 12-13 22-23 23-24 exact bonds : 1-2 1-6 1-32 2-3 2-33 3-4 4-5 5-6 7-15 8-10 10-11 11-14 12-17 21-35 22-31 23-29 26-34 normalized bonds : 16-17 16-21 17-18 18-19 19-20 20-21 25-26 25-30 26-27 27-28 28-29 29-30 isolated ring systems : containing 1 : 16 : 25 : Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS L1STRUCTURE UPLOADED => s l1 SAMPLE SEARCH INITIATED 10:38:22 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -7 TO ITERATE 0 ANSWERS 100.0% PROCESSED 7 ITERATIONS SEARCH TIME: 00.00.03 FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\* \*\*COMPLETE\*\* BATCH PROJECTED ITERATIONS: 7 TO 298 PROJECTED ANSWERS: 0 TO 0 0 SEA SSS SAM L1 1.2 => s 11 ful FULL SEARCH INITIATED 10:38:30 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 191 TO ITERATE 1 ANSWERS 100.0% PROCESSED 191 ITERATIONS SEARCH TIME: 00.00.01 L3 1 SEA SSS FUL L1 => d scan REGISTRY COPYRIGHT 2005 ACS on STN T.3 1 ANSWERS Benzamide, N-[2-[[(1R,2S)-2-[(4-chlorobenzoyl)amino]cyclohexyl]amino]-2-TN oxoethyl]-3-(trifluoromethyl)-, rel- (9CI)

C23 H23 C1 F3 N3 O3

MF

Relative stereochemistry.

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

## ALL ANSWERS HAVE BEEN SCANNED

=> file caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 161.33 161.54

FULL ESTIMATED COST

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FILE COVERS 1907 - 21 Apr 2005 VOL 142 ISS 17 FILE LAST UPDATED: 20 Apr 2005 (20050420/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

#### => d his

(FILE 'HOME' ENTERED AT 10:37:53 ON 21 APR 2005)

FILE 'REGISTRY' ENTERED AT 10:38:01 ON 21 APR 2005

L1 STRUCTURE UPLOADED L2 0 S L1

L2 0 S L1 L3 1 S L1 FUL

## FILE 'CAPLUS' ENTERED AT 10:38:47 ON 21 APR 2005

=> s 13

L4 1 L3

=> d l4 ibib hitstr abs

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2002:594806 CAPLUS

DOCUMENT NUMBER:

137:154762

TITLE:

Preparation of N-[2-(cycloalkylamino)-2-oxoethyl] benzamides and related compounds as modulators of chemokine receptor activity

INVENTOR(S):

Cherney, Robert

PATENT ASSIGNEE(S):

Bristol-Myers Squibb Company, USA

SOURCE:

PCT Int. Appl., 286 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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APPLICATION NO.
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    WO 2002060859
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            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
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PRIORITY APPLN. INFO.:
                                           US 2000-256904P
                                                               P 20001220
                                           US 2001-27644
                                                               A3 20011220
                                           WO 2001-US50252
                                                               W 20011220
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OTHER SOURCE(S): MARPAT 137:154762

IT 445479-10-7P, N-[2-[[cis-2-[(4-Chlorobenzoyl)amino]cyclohexyl]amin o]-2-oxoethyl]-3-(trifluoromethyl)benzamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(chemokine receptor modulator; preparation of [(cycloalkylamino)oxoethyl]ben zamides and related compds. as modulators of chemokine receptor activity)

RN 445479-10-7 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[(4-chlorobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

GΙ

AB Title compds. I [wherein; or pharmaceutically acceptable salts thereof] were prepared as modulators of chemokine receptor activity, especially monocyte chemoattractant protein-1 (MCP-1) (no data). For example, N-tert-butoxycarbonylcyclohexane-(S,S)-1,2-diamine was treated with 4-methylmorpholine and [[3-(trifluoromethyl)benzoyl]amino]acetic acid in DMF to give the amide. Deprotection using TFA in CH2Cl2, followed by sequential addition of Hunig's base, 4-chlorobenzaldehyde, and NaHB(OAc)3, afforded the [(cyclohexylamino)oxoethyl]benzamide II. I are useful for the treatment and prevention of inflammatory disease, allergic and autoimmune diseases, and in particular, rheumatoid arthritis, multiple sclerosis, atherosclerosis and asthma (no data).

. 78
70
1

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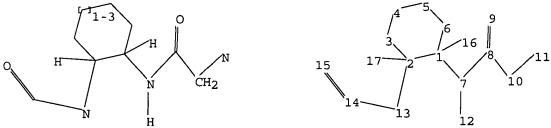
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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chain nodes :

7 8 9 10 11 12 13 14 15 16 17

ring nodes : 1 2 3 4 5

chain bonds :

1-7 1-16 2-13 2-17 7-8 7-12 8-9 8-10 10-11 13-14 14-15

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-7 2-13 7-8 8-9 13-14 14-15

exact bonds :

1-2 1-6 1-16 2-3 2-17 3-4 4-5 5-6 7-12 8-10 10-11 isolated ring systems : containing 1 :

#### Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

L5 STRUCTURE UPLOADED

=> s 15

SAMPLE SEARCH INITIATED 10:47:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 66 TO ITERATE

100.0% PROCESSED 66 ITERATIONS

9 ANSWERS

SEARCH TIME: 00.00.03

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 833 TO 1807 PROJECTED ANSWERS: 9 TO 360

L6 9 SEA SSS SAM L5

=> d scan

L6 9 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]am
ino]-2-oxoethyl]-2-[(2-methyl-2-propenyl)amino]-5-(trifluoromethyl)-, rel(9CI)

MF C27 H32 F3 N5 O5 S

Relative stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.43 173.21

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION
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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 16

L7 3 L6

=> d 17 ibib hitstr abs 1-3

L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:725942 CAPLUS

DOCUMENT NUMBER: 140:209900

TITLE: Design, synthesis and biological evaluation of

ambenonium derivatives as AChE inhibitors

AUTHOR(S): Bolognesi, Maria Laura; Cavalli, Andrea; Andrisano,

Vincenza; Bartolini, Manuela; Banzi, Rita; Antonello,

Alessandra; Rosini, Michela; Melchiorre, Carlo

CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of

Bologna, Bologna, I-40126, Italy Farmaco (2003), 58(9), 917-928

SOURCE: Farmaco (2003), 58(9), 917-928 CODEN: FRMCE8; ISSN: 0014-827X

PUBLISHER: Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal LANGUAGE: English

IT 664338-93-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (design, synthesis and biol. evaluation of ambenonium derivs. as AChE

inhibitors)

RN 664338-93-6 CAPLUS

CN Acetamide, N,N'-(1R,2R)-1,2-cyclohexanediylbis[2-[[(2-chlorophenyl)methyl]ethylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Ambenonium, an old AChE inhibitor, is endowed with an outstanding affinity AB and a peculiar mechanism of action that, taken together, make it a very promising pharmacol. tool for the treatment of Alzheimer's disease (AD). Unfortunately, the bisquaternary structure of ambenonium prevents its passage through the blood brain barrier. In a search of centrally active ambenonium derivs., we planned to synthesize tertiary amines of ambenonium. In addition, to add new insights into the binding mechanism of the inhibitor, we designed constrained analogs of ambenonium by incorporating the diamine functions into cyclic moieties. The biol. evaluation of the new compds. has been assessed in vitro against human AChE and BChE. All tertiary amine derivs. resulted more than 1000-fold less potent than ambenonium and, unlike prototype, did not show any selectivity between the two enzymes. This result, because of recent findings concerning the role of BChE in AD, makes our compds., endowed with a well-balanced profile of AChE/BChE inhibition, valuable candidates for further development. To better clarify the interactions that account for the high affinity of ambenonium, docking simulations and mol. dynamics studies on the AChE-1 complex were also carried out.

19

ACCESSION NUMBER: 2002:594806 CAPLUS

DOCUMENT NUMBER: 137:154762

TITLE: Preparation of N-[2-(cycloalkylamino)-2-

CAPLUS COPYRIGHT 2005 ACS on STN

oxoethyl]benzamides and related compounds as

THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

modulators of chemokine receptor activity

INVENTOR(S): Cherney, Robert

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 286 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

REFERENCE COUNT:

ANSWER 2 OF 3

## PATENT INFORMATION:

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PRIORITY APPLN. INFO.:
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                                                               A3 20011220
                                           WO 2001-US50252
                                                               W 20011220
OTHER SOURCE(S):
                        MARPAT 137:154762
     445479-21-0P, N-[2-[[cis-2-[(4-Trifluoromethoxybenzoyl)amino]cyclo
    hexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-26-5p
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     (trifluoromethyl)benzamide 445479-42-5P, 2-Amino-N-[2-[[cis-2-
     [[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
     chlorobenzamide 445479-49-2P, 4-(Aminosulfonyl)-N-[cis-2-[[[[(3-
    chlorophenyl)sulfonyl]amino]acetyl]amino]cyclohexyl]benzamide
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    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (chemokine receptor modulator; preparation of [(cycloalkylamino)oxoethyl]ben
       zamides and related compds. as modulators of chemokine receptor
       activity)
RN
     445479-21-0 CAPLUS
CN
    Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[4-(trifluoromethoxy)benzoyl]amino]cycl
     ohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)
```

Relative stereochemistry.

RN 445479-26-5 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[(4-methoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-42-5 CAPLUS

CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclo hexyl]amino]-2-oxoethyl]-5-chloro-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-49-2 CAPLUS

CN Benzamide, 4-(aminosulfonyl)-N-[(1R,2S)-2-[[[[(3-chlorophenyl)sulfonyl]amino]acetyl]amino]cyclohexyl]-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-57-2 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(phenylmethyl)amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-65-2 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(2-methyl-2-propenyl)amino]-5-(trifluoromethyl)-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 445479-11-8P, [cis-2-[[[[3-(Trifluoromethyl)benzoyl]amino]acetyl]a mino]cyclohexyl]carbamic acid 1,1-dimethylethyl ester

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of [(cycloalkylamino)oxoethyl]benzamides and related compds. as modulators of chemokine receptor activity)

RN 445479-11-8 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amin o]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

GΙ

AB Title compds. I [wherein; or pharmaceutically acceptable salts thereof] were prepared as modulators of chemokine receptor activity, especially monocyte chemoattractant protein-1 (MCP-1) (no data). For example, N-tert-butoxycarbonylcyclohexane-(S,S)-1,2-diamine was treated with 4-methylmorpholine and [[3-(trifluoromethyl)benzoyl]amino]acetic acid in DMF to give the amide. Deprotection using TFA in CH2Cl2, followed by sequential addition of Hunig's base, 4-chlorobenzaldehyde, and NaHB(OAc)3, afforded the [(cyclohexylamino)oxoethyl]benzamide II. I are useful for the treatment and prevention of inflammatory disease, allergic and autoimmune diseases, and in particular, rheumatoid arthritis, multiple sclerosis, atherosclerosis and asthma (no data).

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:168775 CAPLUS

DOCUMENT NUMBER: 104:168775

TITLE: Amine glycosides and their use INVENTOR(S): Loibner, Hans; Streicher, Wolfgang PATENT ASSIGNEE(S): Sandoz-Patent-G.m.b.H., Fed. Rep. Ger.

SOURCE: Ger. Offen., 10 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
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DE 3445646	A1	19851003	DE 1984-3445646		19841214
PRIORITY APPLN. INFO.:			CH 1984-1444	Α	19840322

IT 101490-82-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and deprotection of)

RN 101490-82-8 CAPLUS

CN L-chiro-Inositol, 1,2,3,6-tetradeoxy-3-[[(1,1dimethylethoxy)carbonyl]amino]-1-[[[[(1,1-dimethylethoxy)carbonyl]amino]ac
etyl]amino]-6-[[[((1,1-dimethylethoxy)carbonyl]amino]acetyl]methylamino]-4O-[2,3,4,6,7-pentadeoxy-2,6-bis[[(1,1-dimethylethoxy)carbonyl]amino]α-D-ribo-heptopyranosyl]- (9CI) (CA INDEX NAME)

GI For diagram(s), see printed CA Issue.

AB Bactericidal (no data) title compds. (I; R1 = H, alkyl; R2 = OH, NH2; R3, R4 = H, OH; R5 = OH, NH2, MeNH; R6 = H, Me; R7 = glycyl) were prepared Thus, 2',3,3'',6'-tetrakis-N-(tert-butoxycarbonyl)gentamicin C2 was oxidized with KMnO4 in aqueous Me2CO to give the 1-deamino-1-nitro derivative which was hydrogenated, N-acylated with a protected glycine derivative, and deprotected to give 6'-epifortimicin derivative II.

=> file req COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 17.97 191.18 TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY SESSION CA SUBSCRIBER PRICE -2.19-2.92

FILE 'REGISTRY' ENTERED AT 10:52:12 ON 21 APR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0 DICTIONARY FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

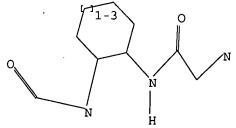
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\107064482.str



chain nodes :

7 8 9 10 11 12 13 14 18

ring nodes :

1 2 3 4 5 6

chain bonds :

1-7 2-12 7-8 7-11 8-9 8-18 10-18 12-13 13-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-7 2-12 7-8 8-9 10-18 12-13 13-14

exact bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-11 8-18

isolated ring systems : containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 18:CLASS

L8 STRUCTURE UPLOADED

=> s 18

SAMPLE SEARCH INITIATED 10:52:32 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -66 TO ITERATE

100.0% PROCESSED

66 ITERATIONS

25 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

833 TO 1807

PROJECTED ANSWERS:

200 TO 800

L9

25 SEA SSS SAM L8

=> d scan

REGISTRY COPYRIGHT 2005 ACS on STN L9 25 ANSWERS

Carbamic acid, [(1R,2R,5S)-2-[[[(5-chloro-2-pyridinyl)amino]oxoacetyl]amin IN o]-5-[(dimethylamino)carbonyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI)

MF C21 H30 Cl N5 O5

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL

FULL ESTIMATED COST	ENTRY 0.43	SESSION 191.61
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY 0.00	SESSION -2.92

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FILE COVERS 1907 - 21 Apr 2005 VOL 142 ISS 17 FILE LAST UPDATED: 20 Apr 2005 (20050420/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> file reg COST IN U.S. DOLLARS	SINCE FILE	TOTAL
,	ENTRY	SESSION
FULL ESTIMATED COST	0.45	192.06
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.92

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STRUCTURE FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0 DICTIONARY FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

\*

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> s 18 ful FULL SEARCH INITIATED 10:53:37 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 1123 TO ITERATE

100.0% PROCESSED 1123 ITERATIONS 481 ANSWERS

SEARCH TIME: 00.00.01

L10 481 SEA SSS FUL L8

=> file caplus COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 161.33 353.39 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -2.92

FILE 'CAPLUS' ENTERED AT 10:53:44 ON 21 APR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 21 Apr 2005 VOL 142 ISS 17 FILE LAST UPDATED: 20 Apr 2005 (20050420/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 110 L11 50 L10

#### => d lll ibib hitstr abs 1-50

L11 ANSWER 2 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:984812 CAPLUS

DOCUMENT NUMBER: 141:415586

TITLE: Preparation of dithiols for hair reinforcement

INVENTOR(S): Philippe, Michel; Andrean, Herve; Barbarat, Philippe

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Eur. Pat. Appl., 18 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

I	PATENT NO.					KIND DATE			APPLICATION NO.						DATE				
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E	ΞP	1477	158			A1		2004	1117	E	P 20	004-	2911	39		2	0040	504	
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB, (	GR,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,	
			ΙE,	SI,	LT,	LV,	FΙ,	RO,	MK,	CY, Z	AL,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	HR
F	FR	2854	797			A1		2004	1119	F	R 20	003-	5899			2	0030	516	
	JP	2004	3392	23		A2		2004	1202	J:	P 20	004-	1456	04		2	0040	514	
J	JS	2005	0192	90		<b>A1</b>		2005	0127	U:	S 20	004-	8466	86		2	0040	517	
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										U	S 20	003-	4777	28P		P 2	0030	612	

OTHER SOURCE(S): MARPAT 141:415586

IT 791592-24-0P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dithiols for hair reinforcement)

RN 791592-24-0 CAPLUS

CN Butanamide, N,N'-1,2-cyclohexanediylbis[2-(acetylamino)-4-mercapto-, (2S,2'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

AB Dithiols such as 2-acetylamino-N-[2-(2-acetylamino-4-mercaptobutyrylamino)ethyl]-4-mercaptobutyramide (I) are useful in formulations for strengthening hair. I was prepared by the reaction of ethylenediamine with homocysteine N-acetylthiolactone in CH2Cl2. A formulation contained I 5-15% and water 7-95%.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:960037 CAPLUS

DOCUMENT NUMBER:

141:400483

TITLE:

Amidic dithiols and their use in hair wave preparations for changing the hair form

INVENTOR(S):

Philippe, Michel; Andrean, Herve

PATENT ASSIGNEE(S):

L'Oreal, Fr.

SOURCE:

Eur. Pat. Appl., 19 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
EP 1475076	A1 20041110	EP 2004-291138	20040504
R: AT, BE, CH,	DE, DK, ES, FR,	GB, GR, IT, LI, LU, NI	L, SE, MC, PT,
IE, SI, LT,	LV, FI, RO, MK,	CY, AL, TR, BG, CZ, EI	E, HU, PL, SK, HR
FR 2854569	A1 20041112	FR 2003-5497	20030506
JP 2004331663	A2 20041125	JP 2004-136487	20040430
US 2005002886	A1 20050106	US 2004-839233	20040506
PRIORITY APPLN. INFO.:		FR 2003-5497	A 20030506
		US 2003-477726P	P 20030612

OTHER SOURCE(S):

MARPAT 141:400483

IT 790227-12-2P

> RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(amidic dithiols and their use in hair wave prepns. for changing hair form)

790227-12-2 CAPLUS RN

Butanamide, N,N'-1,2-cyclohexanediylbis[2-(acetylamino)-4-mercapto- (9CI) CN (CA INDEX NAME)

Preparation of amidic dithiols in hair wave prepns. for changing the hair form ΑB are disclosed. A solution of ethylenediamine in dichloromethane was reacted with a solution of homocysteine N-aceytlthiolactone in dichloromethane to obtain the amidic dithiol of the composition

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS 6 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:802720 CAPLUS

DOCUMENT NUMBER:

141:314159

TITLE:

Preparation of lactam-containing cyclic diamines and derivatives as factor Xa inhibitors for treating

thromboembolic disorders

INVENTOR(S):

Qiao, Jennifer X.; Wang, Tammy C.; Wang, Gren Z.

PATENT ASSIGNEE(S):

Bristol-Myers Squibb Company, USA

SOURCE:

PCT Int. Appl., 260 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.						KIND DATE			APPLICATION NO.							DATE		
							-					<b></b>				-		
	WO 2	004	0826	87		<b>A</b> 1		2004	0930	1	WO 2	004-1	JS80	88		2	0040	317
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								DE,										
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			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
			NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
			TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
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			ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,	SI,
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OTHER SOURCE(S):

MARPAT 141:314159

TT 766552-69-6P, N-(5-Chloropyridin-2-yl)-N'-[(1R,2S)-2-[4-(2-oxo-2H-pyridin-1-yl)benzoylamino]cyclohexyl]oxalamide

RL: PAC (Pharmacological activity): SPN (Synthetic preparation): T

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(factor Xa inhibitor; preparation of lactam-containing cyclic diamines and derivs. as factor Xa inhibitors for treating thromboembolic disorders)

RN 766552-69-6 CAPLUS

CN Ethanediamide, N-(5-chloro-2-pyridinyl)-N'-[(1R,2S)-2-[[4-(2-oxo-1(2H)-pyridinyl)benzoyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

GΙ

Title compds. of formula G-G1-M-Z-A-B [wherein M = central ring selected AB from (un) substituted optionally fused cyclopentane, or cyclohexane, (un) substituted tetrahydropyran, piperidine, piperidin-2-one, pyrrolidine, etc,; G = benzofused ring; G1 = (CH2)1-5 and derivs., (un) substituted CH2:CH2, C(:0), NH, NHCO SO2NH, SO2NHCO, all of the above optionally substituted on one or both ends with alkylene groups, etc., with provisos; Z = NHCO, CONH, Z = (CH2)1-5 and derivs., (un)substituted NHCO, CONH, CO, NHC(:S)NH, S, SO, SO2, SONH, SO2NH, all of the above optionally substituted on one or both ends with alkylene groups, etc.; A = (un) substituted carbo- or heeterocycle; B = lactam or sulfam bound to A ring through an optional linking group attached to the N, pharmaceutically acceptable salts] were prepared as inhibitors of trypsin-like serine proteases, specifically factor Xa, for treating thromboembolic disorders. For example, I was prepared by reductive amination of 4-(2-oxo-2H-pyridin-1yl)benzaldehyde (preparation given) with (1R,2S)-5-Chlorothiophene-2-carboxylic acid (2-aminocyclopentyl) amide in CH2Cl2 in the presence of NaBH(OAc)3/AcOH. Selected invention compds. displayed Ki ≤ 10 μM in a spectrophotometrical assay using purified human factor Xa.

L11 ANSWER 5 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:751590 CAPLUS

DOCUMENT NUMBER:

141:395799

TITLE:

N-tetrachlorophthaloyl (TCP) protection for

solid-phase peptide synthesis

AUTHOR(S):

Cros, Esther; Planas, Marta; Barany, George; Bardaji,

Eduard

CORPORATE SOURCE:

Department of Chemistry, University of Girona, Girona,

17071, Spain

SOURCE:

European Journal of Organic Chemistry (2004), (17),

3633-3642

CODEN: EJOCFK; ISSN: 1434-193X

DOCUMENT TYPE:

Wiley-VCH Verlag GmbH & Co. KGaA Journal

LANGUAGE:

PUBLISHER:

English

IT 787635-14-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(solid-phase peptide synthesis using N-tetrachlorophthaloyl (TCP) protection)

RN 787635-14-7 CAPLUS

CN L-Valinamide, L-phenylalanyl-2-[[(2-aminocyclohexyl)amino]carbonyl]-3,4,5,6-tetrachlorobenzoylqlycyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

AΒ The N-tetrachlorophthaloyl-(TCP-)amino protecting group has been evaluated for use in solid-phase peptide synthesis. The TCP group was unaffected by exposure to either piperidine or N,N-diisopropylethylamine (DIEA), which suggests compatibility with both Fmoc and Boc solid-phase synthesis protocols. Quant. TCP removal was achieved by treatment with hydrazine/DMF (3:17) at 35 °C for 30 min or with ethylenediamine/DMF (1:200) at 50 °C for 30 min. Several C-terminal peptide amides were synthesized successfully by following protocols that use hydrazine/DMF (3:17) at 40 °C for 1 h for repetitive deprotection. Treatment of TCP-amines with methylamine or with diamines did not give the corresponding amines (deprotected), but rather the appropriate N,N'-disubstituted tetrachlorophthalamides, which corresponds to a single ring-opening step. This observation was harnessed to prepare linear and macrocyclic peptide-arene hybrids based on the mild reaction of the parent TCP compound with 1,3-diaminopropane/DMF (1:49) at 25 °C for 5 min.

REFERENCE COUNT:

63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:701975 CAPLUS

DOCUMENT NUMBER:

141:225304

TITLE:

Preparation of cyclohexyl-substituted lactams as

cytokine receptor modulating agents

INVENTOR(S):

Cherney, Robert J.; Carter, Percy; Duncia, John V.;

Gardner, Daniel S.; Santella, Joseph B.

PATENT ASSIGNEE(S):

Bristol-Myers Squibb Company, USA

SOURCE: PC'

PCT Int. Appl., 385 pp.

DOCUMENT TYPE:

CODEN: PIXXD2
Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

. DATE
20040211
Z, AZ, BA, BB, BG, N. CO, CO, CR. CR.

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CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES,
              ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX,
              MZ, MZ, NA, NI
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              BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU,
              MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
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     US 2004186140
                                    20040923
                                                 US 2004-776828
                                                                            20040211
                             Α1
PRIORITY APPLN. INFO.:
                                                 US 2003-446850P
                                                                            20030212
OTHER SOURCE(S):
                            MARPAT 141:225304
     746670-21-3P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (preparation of cyclohexyl-substituted lactams as modulators for cytokine
        receptor activity in the treatment of conditions such as inflammation,
        rheumatoid arthritis, asthma, multiple sclerosis, and atherosclerosis)
RN
     746670-21-3 CAPLUS
     Carbamic acid, [2-[[(2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-4-
CN
     (methylthio) -1-oxobutyl]amino]cyclohexyl] -, phenylmethyl ester (9CI)
```

Absolute stereochemistry.

INDEX NAME)

GΙ

## \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Cyclohexyl-substituted lactams I [A = (un)substituted saturated or partially saturated cycloalkyl or heterocycloalkyl group with 3-8 atoms; E = S(:O)pCHR3, CHR3NR3, C(:O)NR3, N(R3)C(:O)NR3, SO2N(R3), N(R3)SO2N(R3); G = (CHR10)n; J = CH2CH2, CH:CH un(substituted) with (R13)s; R1, R2 = (un)substituted aryl or heteroaryl ring; R3 = H, alkyl; R10 = H, (un)substituted alkyl (two R10 groups may together comprise a carbonyl group); R11, R12 (independently) = H, (un)substituted alkyl, aralkyl, heteroaralkyl, ε-hydroxyalkyl, ε-mercaptoalkyl, ε-alkoxyalkyl, etc.; R13 = H, (un)substituted alkyl; X = O, S; Z = bond, (un)substituted aminocarbonyl, aminothiocarbonyl, aminocarbonylamino, aminothiocarbonyl, aminosulfonylamino, carbonylamino, oxycarbonylamino, aminocarbonyloxy, alkenediyl, methylene, etc.; m = 0-1; n = 0-3; s = 0-1] such as II are prepared as modulators of cytokine activity for the treatment of diseases associated with cytokines and their receptors such as

inflammation, osteo- and rheumatoid arthritis, autoimmune diseases, HIV infection, inflammatory bowel disease, asthma, multiple sclerosis, and atherosclerosis. E.g., 1,4-cyclohexanedione mono(ethylene ketal) is lithiated and acylated with Et cyanoformate, reductively aminated with (S) - $\alpha$ -methylbenzylamine, subjected to reduction with lithium aluminum hydride followed by hydrogenolysis with palladium hydroxide and protection with Cbz anhydride to yield nonracemic III. E.g., III undergoes substitution at the primary carbon with 4-bromophenyl disulfide and tributylphosphine followed by oxidation with mCPBA, Stille methylation of the p-bromophenyl moiety, hydrogenolysis of the Cbz protecting group, acylation with N-Cbz-L-methionine, and S-methylation and cyclization with Me iodide and cesium carbonate to yield IV. E.g., IV undergoes acid-catalyzed deketalization, titanium-mediated Meerwein-Pondorff-Verley reduction with isopropylamine (giving a mixture of both epimers at the amine center), N-methylation with formaldehyde and sodium triacetoxyborohydride, hydrogenolysis of the Cbz protecting group on the aminopyrrolidinone, and acylation with 3-trifluoromethylbenzoic acid and HATU to yield II. The compds. are modulators of chemokine receptor activity (no data). In addition, methods of halolactamization and dehalogenation and reagents appropriate for such transformations are claimed.

L11 ANSWER 8 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:181386 CAPLUS

DOCUMENT NUMBER: 140:385092

TITLE: Physicochemical characterization of the dimeric

lanthanide complexes [en{Ln(DO3A)(H2O)}2] and

[pi{Ln(DTTA)(H2O)}2]2-: A variable-temperature 170 NMR

study

AUTHOR(S): Lee, Tzu-Ming; Cheng, Tsan-Hwang; Ou, Ming-Hung;

Chang, C. Allen; Liu, Gin-Chung; Wang, Yun-Ming

CORPORATE SOURCE: School of Medicinal and Applied Chemistry, Kaohsiung

Medical University, Kaohsiung, 807, Taiwan

SOURCE: Magnetic Resonance in Chemistry (2004), 42(3), 329-336

CODEN: MRCHEG; ISSN: 0749-1581

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

IT

683208-65-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
 (preparation and complexation with lanthanides)

RN 683208-65-3 CAPLUS

CN Glycine, N,N'-[(1R,2R)-1,2-cyclohexanediylbis[imino(2-oxo-2,1-ethanediyl)]]bis[N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)am

ino]ethyl] - (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

PAGE 1-B

∠CO2H

The Gd(III) complexes of the two dimeric ligands [en(DO3A)2] AB {N,N'-bis[1,4,7-tris(carboxymethyl)-1,4,7,10-tetraazacyclododecan-10ylcarbonylmethyl]-N,N'-ethylenediamine} and [pi(DTTA)2]8-[bis(diethylenetriaminepentaacetic acid) diamide derivative with trans-1,2-cyclohexanediamine] were synthesized and characterized. NMR chemical shift of H2O induced by  $[en{Dy(DO3A)}2]$  and  $[pi{Dy(DTTA)}2]2$ - at pH 6.80 proved the presence of 2.1 and 2.2 inner-sphere H2O mols., resp. H2O proton spin-lattice relaxation rates for [en{Gd(DO3A)(H2O)}2] and [pi{Gd(DTTA)(H2O)}2]2- at 37.0  $\pm$  0.1° and 20 MHz are 3.60  $\pm$  0.05 and 5.25  $\pm$  0.05 mM-1 s-1 per Gd, resp. The EPR transverse electronic relaxation rate and 170 NMR transverse relaxation time for the exchange lifetime of the coordinated H2O mol. and the 2H NMR longitudinal relaxation rate of the deuterated diamagnetic La complex for the rotational correlation time were thoroughly studied, and the results were compared with those reported previously for other lanthanide(III) complexes. The exchange lifetimes for  $[en{Gd(DO3A)(H2O)}]2]$  (769 ± 10 ns) and  $[pi\{Gd(DTTA)(H20)\}2]2-(910 \pm 10 ns)$  are significantly higher than those of [Gd(DOTA)(H2O)]- (243 ns) and [Gd(DTPA)(H2O)]2- (303 ns) complexes. The rotational correlation times for [en{Gd(DO3A)(H2O)}2] (150  $\pm$  11 ps) and [pi{Gd(DTTA)(H2O)}2]2- (130  $\pm$  12 ps) are slightly greater than those of [Gd(DOTA)(H2O)]- (77 ps) and [Gd(DTPA)(H2O)]2- (58 ps) complexes. The marked increase in relaxivity (r1) of  $[en{Gd(DO3A)(H2O)}2]$  and  $[pi{Gd(DTTA)(H2O)}2]2$ - result mainly from their longer rotational correlation time and higher mol. weight REFERENCE COUNT: THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS 19

L11 ANSWER 9 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2004:41273 CAPLUS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

DOCUMENT NUMBER:

140:99643

TITLE:

Pharmaceutical compositions comprising novel

anticholinergic agents and NK1-receptor antagonists

for the treatment of respiratory tract diseases

INVENTOR(S):

Pairet, Michel; Meade, Christopher John Montague;

Pieper, Michael P.

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G.,

Germany

SOURCE:

PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.						KIND DATE				APPLICATION NO.									
	WO	2004	00472	24				2004	0115							2	00306	525		
•		W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,		
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,		
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,		
			PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,		
			TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	zw						
		RW:	GH,	GM,	KΕ,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,		
			KG,	ΚZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	ВG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,		
			FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,		
			BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
	DE	1023	0750			A1		2004	0122	1	DE 2	002-3	1023	0750		2	0020	709		
	ΕP	1521	580			A1		2005	0413	]	EP 2	003-	7625	80		2	0030	525		
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,		
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK.			
	US	2004	0488	86		A1		2004	0311	1	JS 2	003-0	6143	52		2	0030	707		
PRIOR	?ITS	APP	LN.	INFO	. :					]	DE 2	002-	1023	0750	1	A 2	0020	709		
										1	JS 2	002-4	4077	58P	I	2	0020	903		
										1	WO 2	003-1	EP66	57	V	1 2	0030	525		

OTHER SOURCE(S):

MARPAT 140:99643

214487-46-4, MEN-11467 IT

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pharmaceutical compns. comprising anticholinergic agents and NK1-receptor antagonists for treatment of respiratory tract diseases)

214487-46-4 CAPLUS RN

1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-CN methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1oxopropyl]amino]cyclohexyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

AB The invention relates to novel pharmaceutical compns. comprising novel anticholinergic agents and NK1-receptor antagonists, method for production and use thereof in the treatment of respiratory diseases. Thus an inhalation capsule contained (microgram/capsule): 2,2-Diphenylpropionic acid scopine ester methobromide 200; N-[2-(3,5-Bis-trifluoromethylphenyl)-ethyl]-2-{4-[(3-hydroxypropyl)methylamino]piperidin-1-yl}-N-methyl-2-phenylacetamide 150; lactose 12150.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2003:971894 CAPLUS

DOCUMENT NUMBER:

140:13077

TITLE:

Antagonizing NK1 receptors inhibits consumption of

substances of abuse

INVENTOR(S):

Olive, Michael Foster; Whistler, Jennifer

PATENT ASSIGNEE(S):

The Regents of the University of California, USA

SOURCE:

PCT Int. Appl., 24 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	PATENT NO.						KIND DATE			APPLICATION NO.						DATE '			
WO	2003	1014	 59		 A1	-	 2003	1211	1	WO 2	 003-1	JS17	 181		20	0030	 529		
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,		
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,		
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,		
		PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,		
		TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW							
	RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,		
		KG,	ΚZ,	MD,	RU,	TJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,		
		FΙ,	FR,	GB,	GR,	HU,	ΙE,	ΙΤ,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,		
		BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG		
PRIORIT	Y APP	LN.	INFO	.:					1	US 2	002-3	3845	61P		P 20	0020	529		
IT 21	4487-	46-4	, ME	N 11	467														
RL	: PAC	(Ph	arma	colo	gica	l ac	tivi	ty);	THU	(Th	erap	euti	c us	e);	BIOL				
(B:	iolog	ical	stu	dy);	USE	S (U	ses)												
	(antagonizing NK1 receptors inhibits consumption of substances of																		

(antagonizing NK1 receptors inhibits consumption of substances of abuse)

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

AB This invention pertains to the surprising discovery that administration of one or more NK1 receptor antagonists to a mammal can inhibit self-administration of a substance of abuse (e.g. alc.). In one embodiment, this invention provides a method of inhibiting or reducing self-administration of a substance of abuse by a mammal. The method involves administering to the mammal an NK1 receptor antagonist in a concentration sufficient to reduce self-administration of a substance of abuse and/or craving for a substance of abuse (e.g. ethanol).

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 11 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2003:737529 CAPLUS

DOCUMENT NUMBER:

139:276714

TITLE:

Preparation of arylthiomethyl carbamoylcyclohexanes

and related compounds as modulators of chemokine

receptor activity

INVENTOR(S):

Cherney, Robert J.

PATENT ASSIGNEE(S):

Bristol-Myers Squibb Company, USA

SOURCE:

PCT Int. Appl., 293 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

					APPLICATION NO.												
						-									-		
WO	2003	0758	53		A2		2003	0918	1	WO 2	003-1	US71	45		2	0030	307
WO	2003	0758	53		A3		2004	0401									
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		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FΙ,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
		PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,
		TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW					
	RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
		KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	ΒE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	SI,	SK,	TR,	BF,
		ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG	
US	2003	2164	34		A1		2003	1120	1	US 2	003-	3833	91		2	0030	307
EP 1483241							2004	1208		EP 2	003-	7140	09		2	0030	307
	R:	ΑT,	ΒE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	LT,	LV,	FΙ,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK	
PRIORITY	Y APP	LN.	INFO	.:					1	US 2	002-	3626	04P	1	P 2	0020	308
						1	WO 2	003-1	US71	45	1	<i>i</i> 2	0030	307			

OTHER SOURCE(S):

MARPAT 139:276714

IT 604765-26-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of arylthiomethyl carbamoylcyclohexanes and related compds. as modulators of chemokine receptor activity)

RN 604765-26-6 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[[[4-(methylthio)phenyl]amino]carbonyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

R1E(CHR13)sB(CHR13)sNR14CO(CR10R10a)nN(R8)ZR2 [B = (unsatd.) (substituted) AB 3-8 membered cycloalkyl, 3-7 membered heterocyclyl; Z = bond, CO, CONH, CSNH, SO2, SO2NH; E = NHCO2, SOpCHR15, COCHR15, etc.; R1, R2 = (substituted) aryl, heteroaryl; R8 = H, alkyl, cycloalkyl; R10, R10a = H, (substituted) alkyl; R13 = Me, (substituted) alkyl; R14, R15 = H, alkyl; n = 1, 2; p = 0-2; s = 0, 1], were prepared as drugs (no data). Thus, (1S\*,2R\*)(2-phenylsulfanylmethylcyclohexyl)carbamic acid tert-Bu ester (preparation given) in CH2Cl2 at 0° was treated with CF3CO2H and the reaction was warmed to rt to give a residue. This in DMF with diisopropylethylamine and BOC-Gly-OH at 0° was treated with BOP followed by warming to room temperature and stirring overnight. The resulting residue was treated with CF3CO2H in CH2Cl2 at 0° to room temperature to give a residue which in DMF with diisopropylethylamine and 2-(tert-butoxycarbonyl)amino-5-trifluoromethylbenzoic acid at 0° was treated with BOP followed by warming to room temperature and stirring overnight to give tert-Bu 2-[[[2-[[(1S\*,2R\*)-2-[(phenylthio)methyl]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl) phenylcarbamate.

L11 ANSWER 12 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:725942 CAPLUS

DOCUMENT NUMBER:

140:209900

TITLE:

Design, synthesis and biological evaluation of

ambenonium derivatives as AChE inhibitors

AUTHOR(S): Bolognesi, Maria Laura; Cavalli, Andrea; Andrisano, Vincenza; Bartolini, Manuela; Banzi, Rita; Antonello,

PUBLISHER:

Alessandra; Rosini, Michela; Melchiorre, Carlo

CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of

Bologna, Bologna, I-40126, Italy

SOURCE: Farmaco (2003), 58(9), 917-928 CODEN: FRMCE8; ISSN: 0014-827X

Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal LANGUAGE: English

IT 664338-93-6P 664338-96-9P 664338-98-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL

(Biological study); PREP (Preparation)

(design, synthesis and biol. evaluation of ambenonium derivs. as AChE

inhibitors)

RN 664338-93-6 CAPLUS

CN Acetamide, N,N'-(1R,2R)-1,2-cyclohexanediylbis[2-[[(2-chlorophenyl)methyl]ethylamino]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 664338-96-9 CAPLUS

CN Acetamide, N,N'-(1S,2S)-1,2-cyclohexanediylbis[2-[[(2-chlorophenyl)methyl]ethylamino]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 664338-98-1 CAPLUS
CN Acetamide, N,N'-(1R,2S)-1,2-cyclohexanediylbis[2-[[(2-chlorophenyl)methyl]ethylamino]-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

AB Ambenonium, an old AChE inhibitor, is endowed with an outstanding affinity and a peculiar mechanism of action that, taken together, make it a very promising pharmacol. tool for the treatment of Alzheimer's disease (AD). Unfortunately, the bisquaternary structure of ambenonium prevents its passage through the blood brain barrier. In a search of centrally active ambenonium derivs., we planned to synthesize tertiary amines of ambenonium. In addition, to add new insights into the binding mechanism of the inhibitor, we designed constrained analogs of ambenonium by incorporating the diamine functions into cyclic moieties. The biol. evaluation of the new compds. has been assessed in vitro against human AChE and BChE. All tertiary amine derivs. resulted more than 1000-fold less potent than ambenonium and, unlike prototype, did not show any selectivity between the two enzymes. This result, because of recent findings concerning the role of BChE in AD, makes our compds., endowed with a well-balanced profile of AChE/BChE inhibition, valuable candidates for further development. To better clarify the interactions that account

for the high affinity of ambenonium, docking simulations and mol. dynamics studies on the AChE-1 complex were also carried out.

REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 13 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2003:610660 CAPLUS

DOCUMENT NUMBER:

139:160766

TITLE:

A method for correlating the preprotachykinin gene

(NKNA) polymorphisms with the efficacy and

compatibility of a pharmaceutically active compounds,

such as NK-1 receptor antagonists

INVENTOR(S):

Foernzler, Dorothee; Hashimoto, Lara; Li, Jia; Luedin,

Eric; Sleight, Andrew; Vankan, Pierre

PATENT ASSIGNEE(S):

F. Hoffmann-La Roche A.-G., Switz.

SOURCE:

PCT Int. Appl., 45 pp.

DOCUMENT TYPE:

CODEN: PIXXD2

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT	NO.	KIN	D DATE	APPLICATION NO.	DATE			
	064685 064685			WO 2003-EP630	20030123			
<b>W</b> :	CO, CR, GM, HR, LS, LT,	CU, CZ, HU, ID, LU, LV,	DE, DK, DM, IL, IN, IS, MA, MD, MG,	BA, BB, BG, BR, BY, DZ, EC, EE, ES, FI, JP, KE, KG, KP, KR, MK, MN, MW, MX, MZ, SK, SL, TJ, TM, TN,	GB, GD, GE, GH, KZ, LC, LK, LR, NO, NZ, OM, PH,			
RW:	GH, GM, KG, KZ, FI, FR,	KE, LS, MD, RU, GB, GR,	TJ, TM, AT, HU, IE, IT,	SL, SZ, TZ, UG, ZM, BE, BG, CH, CY, CZ, LU, MC, NL, PT, SE, GQ, GW, ML, MR, NE,	DE, DK, EE, ES, SI, SK, TR, BF,			
	AT, BE,	CH, DE,	DK, ES, FR,	EP 2003-734685 GB, GR, IT, LI, LU, CY, AL, TR, BG, CZ,	NL, SE, MC, PT,			
	158187	A1		BR 2003-7257 US 2003-354693 EP 2002-1937 WO 2003-EP630	20030130 A 20020131			

## IT 214487-46-4, MEN 11467

RL: ANT (Analyte); PAC (Pharmacological activity); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(NK-1 receptor antagonist; method for correlating preprotachykinin gene (NKNA) polymorphisms with efficacy and compatibility of pharmaceutically active compds., such as NK-1 receptor antagonists)

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

AB The present invention relates to a method for correlating single nucleotide polymorphisms in the preprotachykinin (NKNA) gene with the efficacy and compatibility of a pharmaceutically active compound administered to a human being. The invention further relates to a method for determining the efficacy and compatibility of a pharmaceutically active compound administered to a human being which method comprises determining at least

one single nucleotide polymorphism in the NKNA gene. Said methods are based on determining specific single nucleotide polymorphisms in the NKNA gene and determining the efficacy and compatibility of a pharmaceutically active compound in the human by reference to polymorphism in NKNA. The invention further relates to isolated nucleic acids comprising within their sequence the polymorphisms as defined herein, to nucleic acid primers and oligonucleotide probes capable of hybridizing to such nucleic acids and to a diagnostic kit comprising one or more of such primers and probes for detecting a polymorphism in the NKNA gene, to a pharmaceutical pack comprising neurokinin-1 (NK-1) receptor antagonists and instructions for administration of the drug to human beings tested for the polymorphisms as well as to a computer readable medium with the stored sequence information for the polymorphisms in the NKNA gene.

L11 ANSWER 18 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:869585 CAPLUS

DOCUMENT NUMBER: 137:346202

TITLE: Pharmaceutical compositions based on anticholinergics

and NK1-receptor antagonists for the treatment of

respiratory tract diseases

INVENTOR(S): Pairet, Michel; Pieper, Michael P.; Meade, Christopher

J. M.

PATENT ASSIGNEE(S): Germany

SOURCE: U.S. Pat. Appl. Publ., 18 pp., Cont.-in-part of U.S.

Provisional Ser. NO. 281,653.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002169181	A1	20021114	US 2002-92116	20020306
US 6620438	B2	20030916		
DE 10111058	A1	20020912	DE 2001-10111058	20010308
US 2003212075	A1	20031113	US 2003-419358	20030421
US 6696042	B2	20040224		

US 2004151770 **A**1 20040805 US 2004-763894 20040123 PRIORITY APPLN. INFO.: DE 2001-10111058 20010308 Α US 2001-281653P 20010405 Þ US 2002-92116 A1 20020306 US 2003-419358 A1 20030421

OTHER SOURCE(S): MARPAT 137:346202

214487-46-4, MEN-11467

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

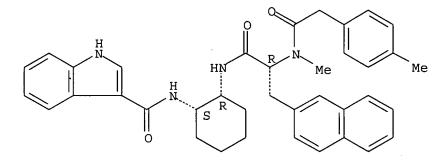
(Biological study); USES (Uses)

(anticholinergics and NK1-receptor antagonists for treatment of respiratory tract diseases)

214487-46-4 CAPLUS RN

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-R)-2-[methyl](4methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1oxopropyl]amino]cyclohexyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



The invention discloses pharmaceutical compns. based on anticholinergics AΒ and NK1-receptor antagonists, processes for preparing them, and their use in the treatment of respiratory tract diseases. Preparation of selected compds. is included.

L11 ANSWER 19 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2002:832668 CAPLUS

DOCUMENT NUMBER:

137:337901

TITLE:

Preparation and use of amides as NK-1 receptor antagonists against benign prostatic hyperplasia

INVENTOR(S):

Buser, Susanne; Ford, Anthony P. D. W.; Hoffmann, Torsten; Lenz, Barbara; Sleight, Andrew John; Vankan,

Pierre

PATENT ASSIGNEE(S):

F. Hoffmann-La Roche A.-G., Switz.

SOURCE:

PCT Int. Appl., 45 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 2002085458 WO 2002085458	A2 20021031 A3 20031030	WO 2002-EP1085	20020202
W: AE, AG, AL,	AM, AT, AU, AZ,	BA, BB, BG, BR, BY, BZ,	
GM, HR, HU,	ID, IL, IN, IS,	DZ, EC, EE, ES, FI, GB, JP, KE, KG, KP, KR, KZ, MK, MN, MW, MX, MZ, NO,	LC, LK, LR,

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PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
             UZ, VN, YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,
             GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,
             GN, GQ, GW, ML, MR, NE, SN, TD, TG
    CA 2444395
                                             CA 2002-2444395
                                                                    20020202
                          AΑ
                                20021031
    EP. 1385577
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                                20040204
                                             EP 2002-719751
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            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                                20040713
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                                             JP 2002-583031
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    US 2003004157
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                          A1
                                20030102
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PRIORITY APPLN. INFO.:
                                             EP 2001-109853
                                                                    20010423
                                             WO 2002-EP1085
                                                                 W
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OTHER SOURCE(S):

MARPAT 137:337901

214487-46-4, MEN 11467 ΙT

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(preparation and use of amides as NK-1 receptor antagonists against benign prostatic hyperplasia)

RN 214487-46-4 CAPLUS

1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-CNmethylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1oxopropyl]amino]cyclohexyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

GΙ

$$\begin{array}{c}
(R^1)_{n} \\
R^2)_{n} \\
R^3 \\
R^3
\end{array}$$

AB Use of an NK-1 receptor antagonist for the treatment or prevention of

benign prostatic hyperplasia (BPH) is claimed. The preferred NK-1 receptor antagonists are compds. of the general formula [I; R = H, alkyl, alkoxy, halo, CF3; R1 = H, halo; RR1 = CH:CHCH:CH; R2, R21 = H, halo CF3, alkyl, alkoxy, cyano; R2R21 = CH:CHCH:CH, optionally substituted by 1-2 alkyl, halo, alkoxy; R3 = H, alkyl; R3R3C = cycloalkyl; R4 = H, N(R5)2, NR5(CH2)nOH, cyclic tertiary amine, etc.; X = CONR5, (CH2)pO, NR5(CH2)p, etc.; R5 = H, cycloalkyl, Ph, PhCH2, alkyl; n = 0-4; p = 1-3]. Preferred compds. are 2-(3,5-bis-trifluoromethyl-phenyl)-N-methyl-N-(6morpholin-4-yl-4-o-tolyl-pyridin-3-yl)isobutyramide, 3-(3,5-bistrifluoromethyl-phenyl)-N-methyl-N-[6-(4-methyl-piperazin-1-yl)-4-o-tolylpyridin-3-yl]isobutyramide, 2-(3,5-bis-trifluoromethyl-phenyl)-N-[6-(1,1dioxo-1\(\lambda\)-thiomorpholin-4-yl)-4-o-tolyl-pyridin-3-yl]-Nmethylisobutyramide, and 2-(3,5-bis-trifluoromethylphenyl)-N-[6-(1,1-dioxo-1\(\frac{1}{4}\)-thiomorpholin-4-yl)-4-(4-fluoro-2-methyl-phenyl)-pyridin-3-yl]-N-methylisobutyramide. Thus, 2-[3,5-bis(trifluoromethyl)phenyl]-N-methyl-N-(6-thiomorpholin-4-yl-4-o-tolylpyridin-3-yl)isobutyramide (preparation given) oxone were stirred 2 days at room temperature to give 2-(3,5-bistrifluoromethylphenyl)-N-[6-(1,1-dioxo-1λ6-thiomorpholin-4-yl)-4-otolylpyridin-3-yl]-N-methylisobutyramide. 2-(3,5-Bistrifluoromethylphenyl)-N-methyl-N-methyl-N-(6-morpholin-4-yl-4-otolylpyridin-3-yl)isobutyramide at 60 mg/kg/day orally in dogs reduced prostate weight by 58% after 39 wk.

L11 ANSWER 20 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2002:695760 CAPLUS

DOCUMENT NUMBER:

137:237717

TITLE:

Inhalant compositions containing anticholinergics and

NK1 receptor antagonists

INVENTOR (S):

Meade, Christopher John Montaque; Pairet, Michel;

Pieper, Michael Paul

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharma K.-G., Germany

SOURCE:

PCT Int. Appl., 42 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE						
WO 2002069944	A2 20020912	WO 2002-EP1987	20020226						
WO 2002069944	A3 20031002								
W: AE, AG, A	AL, AM, AT, AU, AZ,	BA, BB, BG, BR, BY, BZ	, CA, CH, CN,						
CO, CR, C	CU, CZ, DE, DK, DM,	DZ, EC, EE, ES, FI, GB	, GD, GE, GH,						
GM, HR, I	HU, ID, IL, IN, IS,	JP, KE, KG, KP, KR, KZ	, LC, LK, LR,						
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PL, PT, I	RO, RU, SD, SE, SG,	SI, SK, SL, TJ, TM, TN	, TR, TT, TZ,						
	US, UZ, VN, YU, ZA,								
		SL, SZ, TZ, UG, ZM, ZW	. AM. AZ. BY.						
		BE, CH, CY, DE, DK, ES							
		SE, TR, BF, BJ, CF, CG							
	GW, ML, MR, NE, SN,		,,,						
,,		DE 2001-10111058							
		CA 2002-2439915							
		EP 2002-719915							
	· ·	GB, GR, IT, LI, LU, NL	· · · · · · · · · · · · · · · · · · ·						
	LT, LV, FI, RO, MK,		, 5E, MC, FI,						
		JP 2002-569121 20020226							
PRIORITY APPLN. INFO.			<del>-</del>						
PRIORITI APPLIN. INFO.	•	DE 2001-10111058	A 20010308						

WO 2002-EP1987 W 20020226

OTHER SOURCE(S): MARPA

MARPAT 137:237717

IT **214487-46-4**, MEN-11467

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

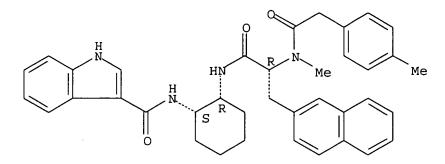
(inhalant compns. containing anticholinergics and NK1 receptor antagonists)

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-

methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB The invention relates to drug compns. based on anticholinergics and on NK1 receptor antagonists, to methods for their production, and to their use as inhalants for the treatment of respiratory tract diseases. Synthesis of NK1 receptor antagonists from the group of bis-trifluoromethyl-phenyl-piperidine derivs. are described. The products are used in suspension aerosols. Thus a composition contained (weight/weight%): tiotropium bromide 0.015:

NK1 receptor antagonist 0.066; soy lecithin 0.2; TG11: TG12 = 2:3 to 100.

L11 ANSWER 21 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:594806 CAPLUS

DOCUMENT NUMBER: 137:154762

TITLE: Preparation of N-[2-(cycloalkylamino)-2-

oxoethyl]benzamides and related compounds as

modulators of chemokine receptor activity

INVENTOR(S): Cherney, Robert

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 286 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.			KIND DATE		APPLICATION NO.						DATE							
WO 2002060859			A2 20020808		WO 2001-US50252						20011220							
WO 2002060859				<b>A</b> 3	A3 20030327													
		<b>W</b> :	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
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			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PH,	PL,
			PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,
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     CA 2432369
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                           A 1
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                                              JP 2002-561010
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                                              US 2003-706448
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PRIORITY APPLN. INFO.:
                                              US 2000-256904P
                                                                      20001220
                                              US 2001-27644
                                                                   A3 20011220
                                              WO 2001-US50252
                                                                   W
                                                                      20011220
OTHER SOURCE(S):
                          MARPAT 137:154762
IT
     445479-24-3P, N-[2-[[cis-2-[(4-Nitrobenzoyl)amino]cyclohexyl]amino
     ]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-47-0P
     445479-62-9P 445480-07-9P, 2-[(Propyl)amino]-N-[2-[[cis-
     2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
     (trifluoromethyl)benzamide 445480-47-7P 445480-49-9P,
     [4-(4-Methylthiobenzoylamino)-3-[[2-(3-trifluoromethylbenzoylamino)acetyl]
     amino]cyclohexyl]carbamic acid benzyl ester 445480-52-4P
     445480-54-6P, 1-(4-Methylthiobenzoylamino)-2-[[2-(3-
     trifluoromethylbenzoylamino)acetyl]amino]-6-aminocyclohexane
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (chemokine receptor modulator; preparation of [(cycloalkylamino)oxoethyl]ben
        zamides and related compds. as modulators of chemokine receptor
        activity)
RN
     445479-24-3 CAPLUS
CN
     Benzamide, N-[2-[[(1R,2S)-2-[(4-nitrobenzoyl)amino]cyclohexyl]amino]-2-
     oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)
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Relative stereochemistry.

RN 445479-47-0 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclo
hexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 445479-46-9 CMF C23 H26 F3 N5 O5 S

$$F_3$$
C

 $NH_2$ 
 $NH_2$ 
 $NH_2$ 
 $NH_2$ 
 $NH_2$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 445479-62-9 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cycloh exyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethoxy)phenyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$H_2N$$
 $R$ 
 $H_2N$ 
 $H_1$ 
 $H_2N$ 
 $H_2N$ 
 $H_1$ 
 $H_2N$ 
 $H_2N$ 
 $H_1$ 
 $H_2N$ 
 $H_2N$ 
 $H_1$ 
 $H_2N$ 
 $H_2N$ 

RN 445480-07-9 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]a mino]-2-oxoethyl]-2-(propylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445480-47-7 CAPLUS

CN Carbamic acid, [3-[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]-4-[[4-(methylthio)benzoyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 445480-49-9 CAPLUS

CN Carbamic acid, [4-[[4-(methylthio)benzoyl]amino]-3-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 445480-52-4 CAPLUS

CN Benzamide, 2-amino-N-[2-[[5-[(1-methylethyl)amino]-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 445480-54-6 CAPLUS

CN Benzamide, N-[2-[[3-amino-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

IT 445479-10-7P, N-[2-[[cis-2-[(4-Chlorobenzoyl)amino]cyclohexyl]amin o]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-12-9P, N-[2-[[cis-2-[(4-Methylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-13-0P, N-[2-[[cis-2-[(4-Fluorobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-14-1P, N-[2-[[cis-2-(Benzoylamino)cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-15-2P, N-[2-[[cis-2-[(4-Bromobenzoyl)amino]cyclohexyl]amino ]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-16-3P, N-[2-[[cis-2-[(4-Phenoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-17-4P, N-[2-[[cis-2-[(4-Trifluoromethylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-18-5P 445479-19-6P, N-[2-[[cis-2-[(4-Iodobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-20-9P, N-[2-[[cis-2-[(4-Cyanobenzoyl) amino] cyclohexyl] amino] -2-oxoethyl] -3-(trifluoromethyl)benzamide 445479-21-0P, N-[2-[[cis-2-[(4-Trifluoromethoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-22-1P, N-[2-[[cis-2-[(4-Formylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-23-2P, N-[2-[[cis-2-[(4-Carbomethoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-25-4P, N-[2-[[cis-2-[(4-Aminobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-26-5P, N-[2-[[cis-2-[(4-Methoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl) benzamide 445479-27-6P, N-[2-[[cis-2-[(4-Methylthiobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide 445479-28-7P, N-[2-[[cis-2-[(4-Methylsulfonylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-

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(trifluoromethyl)benzamide 445479-29-8P, N-[2-[[cis-2-[(4-
Aminosulfonylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-
(trifluoromethyl)benzamide 445479-30-1P, N-[2-[[cis-2-[(4-
Isopropylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-
(trifluoromethyl) benzamide 445479-31-2P, N-[2-[[cis-2-[(4-
Phenylthiobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-
(trifluoromethyl)benzamide 445479-32-3P, N-[2-[[cis-2-[[4-(N,N-
Diethylsulfamoyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-
(trifluoromethyl)benzamide 445479-33-4P, N-[2-[[cis-2-[(4-
Trifluoromethylthiobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-
(trifluoromethyl)benzamide 445479-39-0P, 2-Amino-N-[2-[[cis-2-
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iodobenzamide 445479-42-5P, 2-Amino-N-[2-[[cis-2-[[4-
(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
chlorobenzamide 445479-43-6P, N-[2-[[cis-2-[[4-
(Aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-
chlorobenzamide 445479-44-7P, N-[2-[[cis-2-[[4-
(Aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-
trifluoromethoxybenzamide 445479-45-8P 445479-48-1P,
4-(Aminosulfonyl)-N-[cis-2-[[[[[2-(trifluoromethyl)anilino]carbonyl]amino]
acetyl]amino]cyclohexyl]benzamide 445479-49-2P,
4-(Aminosulfonyl)-N-[cis-2-[[[[(3-chlorophenyl)sulfonyl]amino]acetyl]amino
]cyclohexyl]benzamide 445479-50-5P 445479-52-7P
445479-54-9P 445479-56-1P 445479-57-2P,
2-(Benzylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]a
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2-(Ethylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]am
ino]-2-oxoethyl]-5-trifluoromethylbenzamide 445479-59-4P,
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oxoethyl]-5-bromo benzamide 445479-63-0P, 2-Amino-N-[2-[[cis-2-
[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
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trifluoromethylbenzamide 445479-65-2P, 2-[(2-Methyl-2-
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mino] -2-oxoethyl] -5-trifluoromethylbenzamide 445479-67-4P
445479-69-6P, 2-(Butyl)amino-N-[2-[[cis-2-[[4-
(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
trifluoromethylbenzamide 445479-70-9P, 2-(Propyl)amino-N-[2-
[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
trifluoromethylbenzamide 445479-72-1P 445479-74-3P,
2-[(Aminocarbonyl)amino]-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyc
lohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide 445479-76-5p
  2-(Acetylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl
]amino]-2-oxoethyl]-5-trifluoromethylbenzamide 445479-77-6P,
2-(Methylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]a
mino]-2-oxoethyl]-5-iodobenzamide 445479-78-7P,
2-(Ethylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]am
ino]-2-oxoethyl]-5-iodobenzamide 445479-80-1P
445479-82-3P, 2-Amino-N-[2-[[cis-2-[[4-
(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
nitrobenzamide 445479-83-4P 445479-85-6P
445479-87-8P, 2-(Amino)-N-[2-[[cis-2-[[4-
(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3,5-
dinitrobenzamide 445479-88-9P, 2-[(Isopropylaminocarbonyl)amino]-
N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-
oxoethyl]-5-trifluoromethylbenzamide 445479-89-0P,
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2-[(Cyclohexylcarbonyl)amino]-N-[2-[[cis-2-[[4-
(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
trifluoromethylbenzamide 445479-90-3P, 2-
[(Cyclopentylacetyl)amino] -N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]c
yclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide
445479-91-4P, 2-[(Cyclohexylcarbonyl)amino]-N-[2-[[cis-2-[[4-
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[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
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[(Ethylaminocarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyc
lohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide
445480-16-0P, 2-[(Allylaminocarbonyl)amino]-N-[2-[[cis-2-[[4-
(methylthio) benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
(trifluoromethyl) benzamide 445480-18-2P, 2-
[(Isobutylaminocarbonyl)amino]-N-[2-[[cis-2-[[4-
(methylthio) benzoyl] amino] cyclohexyl] amino] -2-oxoethyl] -5-
(trifluoromethyl) benzamide 445480-21-7P, 2-
[(Cyclopentylaminocarbonyl)amino]-N-[2-[[cis-2-[[4-
(methylthio) benzoyl] amino] cyclohexyl] amino] -2-oxoethyl] -5-
(trifluoromethyl)benzamide 445480-23-9P, 2-[(tert-
Butoxycarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexy
1]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide 445480-24-0P,
2-[(Isopropoxycarbonyl)amino]-N-[2-[[cis-2-[[4-
(methylthio) benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
(trifluoromethyl)benzamide 445480-26-2P, 2-
[(Ethoxycarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohe
xyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide 445480-28-4P
, 2-[(Pyrrolidinylcarbonyl)amino]-N-[2-[[cis-2-[[4-
(methylthio) benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
(trifluoromethyl) benzamide 445480-29-5P, 2-
[(Morpholinylcarbonyl)amino]-N-[2-[[cis-2-[[4-
(methylthio) benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-
(trifluoromethyl)benzamide 445480-31-9P, 2-
[(Azetidinylcarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyc
lohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide
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445480-48-8P 445480-53-5P, 1-(4-Methylthiobenzoylamino)-2-[[2-(2-amino-5-trifluoromethylbenzoylamino)acetyl]amino]-4-(3methylureido) cyclohexane 445480-57-9P 445480-67-1P, 4-(4-Methylthiobenzoylamino)-3-[[2-(3-trifluoromethylbenzoylamino)acetyl]a mino]-4-(2-propylamino)cyclohexane 445480-68-2P, 1-(4-Methylthiobenzoylamino)-2-[[2-(3-trifluoromethylbenzoylamino)acetyl]a mino]-5-aminocyclohexane 445481-22-1P 445481-23-2P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (chemokine receptor modulator; preparation of [(cycloalkylamino)oxoethyl]ben zamides and related compds. as modulators of chemokine receptor activity) RN 445479-10-7 CAPLUS CN Benzamide, N-[2-[[(1R,2S)-2-[(4-chlorobenzoyl)amino]cyclohexyl]amino]-2oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-12-9 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[(4-methylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-13-0 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[(4-fluorobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445479-14-1 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-(benzoylamino)cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-15-2 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[(4-bromobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-16-3 CAPLUS

CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[(4-phenoxybenzoyl)amino]cyclohexyl]amin o]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445479-17-4 CAPLUS

CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[4-(trifluoromethyl)benzoyl]amino]cyclo hexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-18-5 CAPLUS

CN 1H-Benzotriazole-5-carboxamide, N-[(1R,2S)-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, rel-(9CI) (CAINDEX NAME)

Relative stereochemistry.

RN 445479-19-6 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[(4-iodobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445479-20-9 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[(4-cyanobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-21-0 CAPLUS

CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[4-(trifluoromethoxy)benzoyl]amino]cycl ohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-22-1 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[(4-formylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445479-23-2 CAPLUS

CN Benzoic acid, 4-[[[(1R,2S)-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]a mino]cyclohexyl]amino]carbonyl]-, methyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-25-4 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[(4-aminobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-26-5 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[(4-methoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445479-27-6 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-28-7 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]a mino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$F_3$$
C NH NH NH NH NH NH NH NH NH

RN 445479-29-8 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445479-30-1 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(1-methylethyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-31-2 CAPLUS

CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[4-(phenylthio)benzoyl]amino]cyclohexyl ]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-32-3 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-[(diethylamino)sulfonyl]benzoyl]amino]cycl ohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445479-33-4 CAPLUS

CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[4-[(trifluoromethyl)thio]benzoyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-39-0 CAPLUS

CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclo hexyl]amino]-2-oxoethyl]-5-iodo-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-42-5 CAPLUS

CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclo hexyl]amino]-2-oxoethyl]-5-chloro-, rel- (9CI) (CA INDEX NAME)

RN 445479-43-6 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-chloro-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-44-7 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethoxy)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-45-8 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cycloh exyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

RN 445479-48-1 CAPLUS

CN Benzamide, 4-(aminosulfonyl)-N-[(1R,2S)-2-[[[[[[2-(trifluoromethyl)phenyl]amino]carbonyl]amino]acetyl]amino]cyclohexyl]-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-49-2 CAPLUS

CN Benzamide, 4-(aminosulfonyl)-N-[(1R,2S)-2-[[[[(3-chlorophenyl)sulfonyl]amino]acetyl]amino]cyclohexyl]-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-50-5 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cycloh exyl]amino]-2-oxoethyl]amino]carbonyl]-4-iodophenyl]-, ethyl ester, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-52-7 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cycloh exyl]amino]-2-oxoethyl]amino]carbonyl]-4-iodophenyl]-, methyl ester, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

$$H_2N$$
 $R$ 
 $H_2N$ 
 $H_2N$ 
 $H_1$ 
 $H_1$ 
 $H_2$ 
 $H_2$ 
 $H_1$ 
 $H_2$ 
 $H_1$ 
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 $H_1$ 
 $H_2$ 
 $H_3$ 
 $H_4$ 
 $H_4$ 
 $H_4$ 
 $H_5$ 
 $H_5$ 
 $H_6$ 
 $H_7$ 
 $H_8$ 
 $H_8$ 

RN 445479-54-9 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cycloh exyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]methyl-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

$$H_2N$$
 $R$ 
 $S$ 
 $H$ 
 $O$ 
 $Me$ 
 $NH$ 
 $CF_3$ 
 $CF_3$ 

RN 445479-56-1 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cycloh exyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, ethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-57-2 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(phenylmethyl)amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-58-3 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(ethylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-59-4 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(methylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-61-8 CAPLUS

CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclo hexyl]amino]-2-oxoethyl]-5-bromo-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-63-0 CAPLUS

CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclo hexyl]amino]-2-oxoethyl]-5-(trifluoromethoxy)-, rel- (9CI) (CA INDEX NAME) Relative stereochemistry.

RN 445479-64-1 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(2-propenylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-65-2 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(2-methyl-2-propenyl)amino]-5-(trifluoromethyl)-, rel-(9CI) (CA INDEX NAME)

RN 445479-67-4 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(cyclopropylmethylene)amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry unknown.

$$H_2N$$
 $S$ 
 $H_1$ 
 $H_2$ 
 $H_2$ 
 $H_3$ 
 $H_4$ 
 $H_4$ 

RN 445479-69-6 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(butylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-70-9 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(propylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445479-72-1 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(2-methylpropyl)amino]-5-(trifluoromethyl)-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-74-3 CAPLUS

CN Benzamide, 2-[(aminocarbonyl)amino]-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

$$H_2N$$
 $R$ 
 $H_2N$ 
 $O$ 
 $H_2N$ 
 $O$ 
 $H_2N$ 
 $O$ 
 $O$ 

RN 445479-76-5 CAPLUS

CN Benzamide, 2-(acetylamino)-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-77-6 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-iodo-2-(methylamino)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-78-7 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(ethylamino)-5-iodo-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-80-1 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-iodo-2-[(trifluoroacetyl)amino]-, rel- (9CI) (CA INDEX NAME)

$$H_2N$$
 $R$ 
 $H_2N$ 
 $H_3C$ 
 $H_3$ 

RN 445479-82-3 CAPLUS

CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclo hexyl]amino]-2-oxoethyl]-5-nitro-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 445479-83-4 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cycloh exyl]amino]-2-oxoethyl]amino]carbonyl]-4-iodophenyl]-, 1-methylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-85-6 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cycloh exyl]amino]-2-oxoethyl]amino]carbonyl]-4-iodophenyl]-, 1,1-dimethylethyl

ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$H_2N$$
 $R$ 
 $H_2N$ 
 $H_2N$ 
 $H_1$ 
 $H_2N$ 
 $H_1$ 
 $H_2N$ 
 $H_1$ 
 $H_2$ 
 $H_1$ 
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 $H_7$ 
 $H_8$ 
 $H$ 

RN 445479-87-8 CAPLUS

CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclo hexyl]amino]-2-oxoethyl]-3,5-dinitro-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$H_2N$$
 $R$ 
 $NH$ 
 $NH$ 
 $NH_2$ 
 $NO_2$ 
 $NO_2$ 

RN 445479-88-9 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

$$H_2N$$
 $R$ 
 $H_1$ 
 $H_2N$ 
 $i-PrNH$ 
 $O$ 
 $i-PrNH$ 

RN 445479-89-0 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(cyclohexylcarbonyl)amino]-5-(trifluoromethyl)-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-90-3 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(cyclopentylacetyl)amino]-5-(trifluoromethyl)-, rel-(9CI) (CA INDEX NAME)

RN 445479-91-4 CAPLUS

CN Benzamide, 2-[(cyclohexylcarbonyl)amino]-N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-96-9 CAPLUS

CN Benzamide, 2-[(cyclohexylcarbonyl)amino]-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445479-97-0 CAPLUS

CN Benzamide, 2-[[[(1-methylethyl)amino]carbonyl]amino]-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-98-1 CAPLUS

CN Benzamide, 2-[[[(1-methylethyl)amino]carbonyl]amino]-N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445479-99-2 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(methylsulfonyl)amino]-5-(trifluoromethyl)-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-01-3 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]a mino]-2-oxoethyl]-2-(2-propenylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445480-04-6 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(2-propenylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-05-7 CAPLUS

CN Benzamide, 2-[(2-methyl-2-propenyl)amino]-N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-06-8 CAPLUS

CN Benzamide, 2-[(2-methyl-2-propenyl)amino]-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel-(9CI) (CA INDEX NAME)

RN 445480-08-0 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(propylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-09-1 CAPLUS

CN Benzamide, 2-[(2-methylpropyl)amino]-N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-10-4 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[[[2-[(2-methyl-2-propenyl)amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-,

1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me NH O HN OBU-t
$$H_{2}C$$

$$CF_{3}$$

$$R$$

$$R$$

445480-11-5 CAPLUS RN

CNBenzamide, 2-[(2-methylpropyl)amino]-N-[2-[[(1R,2S)-2-[[4-(methylthio) benzoyl] amino] cyclohexyl] amino] -2-oxoethyl] -5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN

445480-12-6 CAPLUS Benzamide, 2-(butylamino)-N-[2-[[(1R,2S)-2-[[4-CN (methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-13-7 CAPLUS

CN Benzamide, 2-(butylamino)-N-[2-[[(1R,2S)-2-[[4-(methylthio) benzoyl] amino] cyclohexyl] amino] -2-oxoethyl] -5-

(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-14-8 CAPLUS

CN Benzamide, 2-[[(ethylamino)carbonyl]amino]-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-16-0 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino ]-2-oxoethyl]-2-[[(2-propenylamino)carbonyl]amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

445480-18-2 CAPLUS RN

CN(methylthio) benzoyl] amino] cyclohexyl] amino] -2-oxoethyl] -5-(trifluoromethyl) -, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN

445480-21-7 CAPLUS
Benzamide, 2-[[(cyclopentylamino)carbonyl]amino]-N-[2-[[(1R,2S)-2-[[4-CN(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

RN 445480-23-9 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexy l]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, l,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-24-0 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexy l]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, l-methylethyl ester, rel- (9CI) (CA INDEX NAME)

RN 445480-26-2 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexy l]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, ethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-28-4 CAPLUS

CN 1-Pyrrolidinecarboxamide, N-[2-[[[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, rel-(9CI) (CA INDEX NAME)

RN 445480-29-5 CAPLUS

CN 4-Morpholinecarboxamide, N-[2-[[[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-31-9 CAPLUS

CN 1-Azetidinecarboxamide, N-[2-[[[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, rel- (9CI) (CA INDEX NAME)

RN 445480-48-8 CAPLUS

CN Benzamide, N-[2-[[5-amino-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 445480-53-5 CAPLUS

CN Benzamide, 2-amino-N-[2-[[5-[(aminocarbonyl)methylamino]-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 445480-57-9 CAPLUS

CN Benzamide, N-[2-[[3-[(1-methylethyl)amino]-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 445480-67-1 CAPLUS

CN Benzamide, N-[2-[[2-[[4-(methylthio)benzoyl]amino]-5-(propylamino)cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH-C} & \text{SMe} \\ & \text{NH-C} & \text{CH}_2\text{-NH-C} \\ & \text{NH-C} & \text{CH}_2\text{-NH-C} \\ \end{array}$$

RN 445480-68-2 CAPLUS

CN Benzamide, N-[2-[[4-amino-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{NH} & \text{C} & \text{SMe} \\ \hline & \text{NH} & \text{C} & \text{CH}_2 - \text{NH} - \text{C} \\ \hline & \text{O} & \text{CF}_3 \\ \end{array}$$

RN 445481-22-1 CAPLUS

CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[[[4-(methylthio)phenyl]amino]carbony l]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445481-23-2 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[[[4-(methylsulfonyl)phenyl]amino]carb onyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4- (trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

CN

Relative stereochemistry.

```
445478-72-8P, [(1S,2S)-2-[[[[3-(Trifluoromethyl)benzoyl]amino]acet
IT
    yl]amino]cyclohexyl]carbamic acid 1,1-dimethylethyl ester
    445479-11-8P, [cis-2-[[[[3-(Trifluoromethyl)benzoyl]amino]acetyl]a
    mino]cyclohexyl]carbamic acid 1,1-dimethylethyl ester 445479-40-3P
    , Benzyl cis-[2-[[2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-
    oxoethyl]carbamate 445479-41-4P, N-cis-[2-
     [(Aminoacetyl)amino]cyclohexyl]-4-(aminosulfonyl)benzamide hydrobromide
     445479-93-6P 445479-94-7P, [cis-2-[[[[[2-(tert-
    Butyloxycarbonylamino) -5-trifluoromethyl]benzoyl]amino]acetyl]amino]cycloh
     exyl]carbamic acid benzyl ester 445480-02-4P
     445480-03-5P 445480-15-9P, 2-(Amino)-N-[2-[[cis-2-[[4-
     (methylthio) benzoyl] amino] cyclohexyl] amino] -2-oxoethyl] -5-
     (trifluoromethyl) benzamide 445480-20-6P 445480-55-7P,
     [5-Benzyloxycarbonylamino-2-[[2-(3-trifluoromethylbenzoylamino)acetyl]amin
     o]cyclohexyl]carbamic acid tert-butyl ester 445480-56-8P,
     [3-(4-Methylthiobenzoylamino)-4-[[2-(3-trifluoromethylbenzoylamino)acetyl]
    amino]cyclohexyl]carbamic acid benzyl ester 445480-63-7P,
     [4-Benzyloxycarbonylamino-2-[2-[((2-(tert-butoxycarbonylamino)-5-
     (trifluoromethyl)benzoyl)amino)acetyl]amino]cyclohexyl]carbamic acid
     tert-butyl ester 445480-65-9P, [3-[[2-(2-Amino-5-
     trifluoromethylbenzoylamino)acetyl]amino]-4-(4-
    methylsulfanylbenzoylamino)cyclohexyl]carbamic acid benzyl ester
     445480-66-0P, [4-Benzyloxycarbonylamino-2-[[2-(3-
     trifluoromethylbenzoylamino)acetyl]amino]cyclohexyl]carbamic acid
     tert-butyl ester 445480-71-7P, cis-[2-[[2-(2-Isopropylamino-5-
     trifluoromethylbenzoylamino)acetyl]amino]cyclohexyl]carbamic acid
     tert-butyl ester 445480-73-9P 445480-75-1P
     445481-13-0P, [5-Benzyloxy-2-[[2-(3-trifluoromethylbenzoylamino)ac
     etyl]amino]cyclohexyl]carbamic acid tert-butyl ester 445481-14-1P
     , [5-Azido-2-[[2-(3-trifluoromethylbenzoylamino)acetyl]amino]cyclohexyl]ca
     rbamic acid tert-butyl ester
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (intermediate; preparation of [(cycloalkylamino)oxoethyl]benzamides and
        related compds. as modulators of chemokine receptor activity)
     445478-72-8 CAPLUS
RN
```

Carbamic acid, [(1S,2S)-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amin

o]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 445479-11-8 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amin o]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-40-3 CAPLUS

CN Carbamic acid, [2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl] amino]-2-oxoethyl]-, phenylmethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$H_2N$$
 $H_2N$ 
 $H_1$ 
 $H_2N$ 
 $H_1$ 
 $H_2$ 
 $H_3$ 
 $H_4$ 
 $H_4$ 
 $H_5$ 
 $H_6$ 
 $H_7$ 
 $H_8$ 
 $H_8$ 
 $H_1$ 
 $H_1$ 
 $H_1$ 
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 $H_1$ 
 $H_2$ 
 $H_3$ 
 $H_4$ 
 $H_1$ 
 $H_2$ 
 $H_3$ 
 $H_4$ 
 $H$ 

RN 445479-41-4 CAPLUS

CN Benzamide, N-[(1R,2S)-2-[(aminoacetyl)amino]cyclohexyl]-4-(aminosulfonyl)-, monohydrobromide, rel- (9CI) (CA INDEX NAME)

HBr

RN 445479-93-6 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[[[(1,1-dimethylethoxy)carbonyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445479-94-7 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-02-4 CAPLUS

CN Carbamic acid, [2-[[(1R,2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]cyclohe xyl]amino]-2-oxoethyl]-, phenylmethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-03-5 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[[[2-(2-propenylamino)-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-15-9 CAPLUS

CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohex yl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-20-6 CAPLUS

CN Carbamic acid, [2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

RN 445480-55-7 CAPLUS

CN Carbamic acid, [3-[[(1,1-dimethylethoxy)carbonyl]amino]-4-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 445480-56-8 CAPLUS

CN Carbamic acid, [3-[[4-(methylthio)benzoyl]amino]-4-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 445480-63-7 CAPLUS

CN Carbamic acid, [4-[[(1,1-dimethylethoxy)carbonyl]amino]-3-[[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 445480-65-9 CAPLUS

CN Carbamic acid, [3-[[[2-amino-5-(trifluoromethyl)benzoyl]amino]acetyl]amin o]-4-[[4-(methylthio)benzoyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 445480-66-0 CAPLUS

CN Carbamic acid, [4-[[(1,1-dimethylethoxy)carbonyl]amino]-3-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 445480-71-7 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[[[2-[(1-methylethyl)amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

RN 445480-73-9 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[[[2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-,
1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 445480-75-1 CAPLUS

CN Carbamic acid, [2-[[[2-[(4-morpholinylcarbonyl)amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 445481-13-0 CAPLUS

CN Carbamic acid, [5-(phenylmethoxy)-2-[[[[3-(trifluoromethyl)benzoyl]amino]a cetyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 445481-14-1 CAPLUS

CN Carbamic acid, [5-azido-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amin o]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

GΙ

AB Title compds. I [wherein; or pharmaceutically acceptable salts thereof] were prepared as modulators of chemokine receptor activity, especially monocyte chemoattractant protein-1 (MCP-1) (no data). For example, N-tert-butoxycarbonylcyclohexane-(S,S)-1,2-diamine was treated with 4-methylmorpholine and [[3-(trifluoromethyl)benzoyl]amino]acetic acid in DMF to give the amide. Deprotection using TFA in CH2Cl2, followed by sequential addition of Hunig's base, 4-chlorobenzaldehyde, and NaHB(OAc)3, afforded the [(cyclohexylamino)oxoethyl]benzamide II. I are useful for the treatment and prevention of inflammatory disease, allergic and autoimmune diseases, and in particular, rheumatoid arthritis, multiple

sclerosis, atherosclerosis and asthma (no data).

L11 ANSWER 22 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:484021 CAPLUS

DOCUMENT NUMBER: 137:379900

TITLE: Pharmacology of MEN 11467: a potent new selective and

orally-effective peptidomimetic tachykinin NK1

receptor antagonist

AUTHOR(S): Cirillo, R.; Astolfi, M.; Conte, B.; Lopez, G.;

Parlani, M.; Sacco, G.; Terracciano, R.; Fincham, C. I.; Sisto, A.; Evangelista, S.; Maggi, C. A.; Manzini,

S.

CORPORATE SOURCE: Department of Pharmacology, Menarini Ricerche SpA,

Pomezia-Roma, I-00040, Italy

SOURCE: Neuropeptides (Edinburgh, United Kingdom) (2001),

35(3&4), 137-147

CODEN: NRPPDD; ISSN: 0143-4179

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

IT 214487-46-4, MEN 11467

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU

(Therapeutic use); BIOL (Biological study); USES (Uses)

(pharmacol. of a potent new selective and orally-effective peptidomimetic tachykinin NK1 receptor antagonist, MEN 11467)

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-

oxopropyl]amino]cyclohexyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

We have investigated the pharmacol. properties of MEN 11467, a novel partially retro-inverse peptidomimetic antagonist of tachykinin NK1 receptors. MEN 11467 potently inhibits the binding of [3H] substance P (SP) to tachykinin NK1 receptors in the IM9 limphoblastoid cell line (pKi = 9.4±0.1). MEN 11467 is highly specific for the human tachykinin NK1 receptors, since it has negligible effects (pKi <6) on the binding of specific ligands to tachykinin NK2 or NK3 receptors and to a panel of 30 receptors ion channels unrelated to tachykinin receptors. The antagonism exerted by MEN 11467 at tachykinin NK1 receptors is insurmountable in saturation binding expts., both KD and Bmax of SP were significantly reduced by MEN 11467 (0.3-10 nM). In the guinea-pig isolated ileum, MEN 11467

(0.03-1 nM) produced a nonparallel rightward shift of the

concentration-response

curve to SP methylester with a concomitant reduction of the Emax to the agonist (pKB =  $10.7\pm0.1$ ). Moreover the antagonist activity of MEN

11467 was hardly reversible despite prolonged washout. In vivo, MEN 11467 produced a long lasting (> 2-3 h) dose-dependent antagonism of bronchoconstriction induced by the selective tachykinin NK1 receptor agonist, [Sar9, Met(O2)11]SP in anesthetized guinea-pigs (ID50s' =  $29\pm5$ ,  $31\pm12$  and  $670\pm270$   $\mu g/kg$ , after i.v., intranasal and intraduodenal administration, resp.), without affecting bronchoconstriction induced by methacholine. After oral administration MEN 11467 produced a dose-dependent inhibition of plasma protein extravasation induced in guinea-pig bronchi by [Sar9, Met(O2)11] (ID50 =  $6.7\pm2$  mg/kg) or by antigen challenge in sensitized animals (ID50 = 1.3mg/kg). After i.v. administration MEN 11467 weakly inhibited the GR 73632-induced foot tapping behavior in gerbil (ED50 =  $2.96\pm2$  mg/kg), indicating a poor ability to block central tachykinin NK1 receptors. These results demonstrate that MEN 11467 is a potent, highly selective and orally effective insurmountable pseudopeptide antagonist of peripheral tachykinin NK1 receptors with a long duration of action.

REFERENCE COUNT:

THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 23 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

32

ACCESSION NUMBER: 2002:311304 CAPLUS

DOCUMENT NUMBER: 137:149471

TITLE: New CSPs based on peptidomimetics: efficient chiral

selectors in enantioselective separations

AUTHOR(S): Burguete, M. Isabel; Frechet, Jean M. J.;

Garcia-Verdugo, Eduardo; Janco, Miroslav; Luis, Santiago V.; Svec, Frantisek; Vicent, Maria J.; Xu,

Mingcheng

CORPORATE SOURCE: Department of Inorganic and Organic Chemistry,

E.S.T.C.E. Universitat Jaume I, Castellon, E-12080,

Spain

SOURCE: Polymer Bulletin (Berlin, Germany) (2002), 48(1), 9-15

CODEN: POBUDR; ISSN: 0170-0839

PUBLISHER: Springer-Verlag

DOCUMENT TYPE: Journal LANGUAGE: English

IT 444891-04-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in preparation of chiral stationary phases based on peptidomimetics for enantioselective sepns.)

RN 444891-04-7 CAPLUS

CN Benzenepropanamide, N,N'-(1S,2S)-1,2-cyclohexanediylbis[ $\alpha$ -amino-, ( $\alpha$ S, $\alpha$ 'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## IT 444647-78-3P

RL: ARU (Analytical role, unclassified); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent)

(peptidomimetics; preparation of chiral stationary phases based on peptidomimetics for enantioselective sepns.)

RN 444647-78-3 CAPLUS

CN Benzenepropanamide, N,N'-(1S,2S)-1,2-cyclohexanediylbis [ $\alpha$ -[(2-methyl-1-oxo-2-propenyl)amino]-, ( $\alpha$ S, $\alpha$ 'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## IT 444647-82-9P 444647-83-0P

RL: ARU (Analytical role, unclassified); NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(preparation of chiral stationary phases based on peptidomimetics for enantioselective sepns.)

RN 444647-82-9 CAPLUS

CN Benzenepropanamide, N,N'-(1S,2S)-1,2-cyclohexanediylbis[ $\alpha$ -[(2-methyl-1-oxo-2-propenyl)amino]-, ( $\alpha$ S, $\alpha$ 'S)-, polymer with diethenylbenzene and ethenylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 444647-78-3 CMF C32 H40 N4 O4

Absolute stereochemistry.

CM 2

CRN 1321-74-0 CMF C10 H10 CCI IDS



CM 3

CRN 100-42-5 CMF C8 H8

# $H_2C = CH - Ph$

RN 444647-83-0 CAPLUS

CN 2-Propenoic acid, 2-methyl-, 2-ethyl-2-[[(2-methyl-1-oxo-2-propenyl)oxy]methyl]-1,3-propanediyl ester, polymer with methyl 2-methyl-2-propenoate and (αS,α'S)-N,N'-(1S,2S)-1,2-cyclohexanediylbis[α-[(2-methyl-1-oxo-2-propenyl)amino]benzenepropanamide] (9CI) (CA INDEX NAME)

CM 1

CRN 444647-78-3 CMF C32 H40 N4 O4

Absolute stereochemistry.

CM 2

CRN 3290-92-4

CMF C18 H26 O6

CM 3

CRN 80-62-6 CMF C5 H8 O2

AB Two different families of peptidomimetics were synthesized and used as chiral selectors for enantioselective chromatog. The functionalization of compds. with multiple nitrogen atoms allows their use in the preparation of chiral stationary phases (CSPs), with acrylic or styril comonomers, in both bead and monolithic formats. Some of these separation media, having the appropriate morphol. properties for their use in chromatog. columns, were able to efficiently discriminate enantiomers of amino acid derivs. and pharmaceuticals such as oxazepam.

REFERENCE COUNT:

THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 24 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

36

ACCESSION NUMBER: 2001:923610 CAPLUS

DOCUMENT NUMBER: 136:31709

TITLE: Method of treating symptoms of hormonal variation,

including hot flashes, using a tachykinin receptor

antagonist

INVENTOR(S): Guttuso, Thomas J., Jr.

PATENT ASSIGNEE(S): University of Rochester, USA

SOURCE: PCT Int. Appl., 19 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT	NO.			KIN	D	DATE		1	APPL	ICAT	ION	NO.		D	ATE	
					_									-		
WO 2001095904			A1 20011220		WO 2001-US40924					20010612						
W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,
	HU,	ID,	IL,	IN,	IS,	JΡ,	KΕ,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,
	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	ΡL,	PT,	RO,	RU,
	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	UΖ,	VN,	YU,
	ZA,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM					

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG 20011220 CA 2001-2412355 20010612 CA 2412355 AΑ US 2001-879390 US 2002016283 A1 20020207 20010612 EP 2001-942248 20010612 EP 1299100 A1 20030409 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR US 2003-609176 20030627 20031225 US 2003236237 A1 20000612 US 2000-211116P Р PRIORITY APPLN. INFO.: US 2001-879390 A1 20010612 WO 2001-US40924 20010612

IT 214487-46-4, MEN 11467

> RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(tachykinin receptor antagonist for treating symptoms of hormonal variation, including hot flashes)

214487-46-4 CAPLUS RN

1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-CNmethylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1oxopropyl]amino]cyclohexyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Methods are provided for treating hot flashes and symptoms of hormonal AB variation in a patient, which methods include providing a tachykinin receptor antagonist and administering the tachykinin receptor antagonist to a patient experiencing a symptom of hormonal variation under conditions effective to treat the symptom of hormonal variation, which symptoms of hormonal variation can include hot flashes.

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 25 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

2001:523530 CAPLUS ACCESSION NUMBER:

135:111983 DOCUMENT NUMBER:

NK1-Receptor antagonists for the treatment of the TITLE:

restless leg syndrome

Brecht, Hans-Michael; Jung, Birgit INVENTOR(S):

Boehringer Ingelheim Pharma K.-G., Germany PATENT ASSIGNEE(S):

Ger. Offen., 4 pp. SOURCE:

CODEN: GWXXBX

Patent DOCUMENT TYPE: German LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10001785	A1	20010719	DE 2000-10001785	20000118
WO 2001052854	A1	20010726	WO 2001-EP263	20010111
W: CA, JP, MX,				
RW: AT, BE, CH,	CY, DE	, DK, ES, FI	, FR, GB, GR, IE, IT,	, LU, MC, NL,
PT, SE, TR				
US 2001034320	A1	20011025	US 2001-764629	20010118
PRIORITY APPLN. INFO.:			DE 2000-10001785	A 20000118
			US 2000-180399P	P 20000204

IT 214487-46-4, MEN 11467

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (NK1-receptor antagonists for treatment of restless leg syndrome)

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

The invention concerns the use from NK1-receptor antagonists for the production of a drug for the treatment of the restless leg syndrome. The drugs are selected from e.g., Neuronorm, BIF 1149, FK 888, SR 48968, SR 140333, and LY 303870. Opioids,  $\alpha 2$ -adrenoceptor agonists, and Antiparkinsonian agents may be used in conjunction with NK1-receptor antagonists.

L11 ANSWER 26 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:457135 CAPLUS

DOCUMENT NUMBER: 135:256988

TITLE: A practical and efficient synthesis of chiral

N,N-disubstituted C2 symmetric diamines derived from

(R,R)-1,2-diaminocyclohexane

AUTHOR(S): Alexakis, A.; Chauvin, A.-S.; Stouvenel, R.; Vrancken,

E.; Mutti, S.; Mangeney, P.

CORPORATE SOURCE: Department of Organic Chemistry, University of Geneva,

Geneva, CH-1211, Switz.

SOURCE: Tetrahedron: Asymmetry (2001), 12(8), 1171-1178

CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:256988

IT 361382-28-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(N-alkylation of diaminocyclohexane)

RN361382-28-7 CAPLUS

Acetamide, N,N'-(1R,2R)-1,2-cyclohexanediylbis[2-(dimethylamino)- (9CI) CN (CA INDEX NAME)

Absolute stereochemistry.

An improved synthesis of chiral diamine ligands derived from AB (R,R)-1,2-diaminocyclohexane is described, providing N-substituted The synthesis of other new ligands based on this methodol. is also reported.

REFERENCE COUNT:

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS 21 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 27 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2001:271293 CAPLUS

DOCUMENT NUMBER:

134:367567

TITLE:

Synthesis of soluble complexan polymers in organic

solvents for using as a polymer-chelate precursor to

YBa2Cu3O7-x thin films

AUTHOR (S):

Naka, Kensuke; Tanaka, Yasuyuki; Yamasaki, Kunitoshi;

Ohki, Akira; Chujo, Yoshiki; Maeda, Shigeru

CORPORATE SOURCE:

Department of Polymer Chemistry, Graduate School of Engineering, Kyoto university, Kyoto, 606-8501, Japan

SOURCE:

TΤ

Bulletin of the Chemical Society of Japan (2001),

74(3), 571-577

CODEN: BCSJA8; ISSN: 0009-2673

PUBLISHER:

Chemical Society of Japan

DOCUMENT TYPE:

Journal

English

LANGUAGE:

340320-89-0DP, metal complexes

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis of soluble complex polymers in organic solvents for using as a

polymer-chelate precursor to YBa2Cu3O7-x thin films)

340320-89-0 CAPLUS RN

Poly[[(carboxymethyl)imino]-(1R,2R)-1,2-cyclohexanediyl[(carboxymethyl)imi CNno](2-oxo-1,2-ethanediyl)imino-(1R,2R)-1,2-cyclohexanediylimino(1-oxo-1,2ethanediyl)], rel- (9CI) (CA INDEX NAME)

IT 340320-89-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of soluble complex polymers in organic solvents for using as a polymer-chelate precursor to YBa2Cu3O7-x thin films)

RN 340320-89-0 CAPLUS

CN Poly[[(carboxymethyl)imino]-(1R,2R)-1,2-cyclohexanediyl[(carboxymethyl)imino](2-oxo-1,2-ethanediyl)imino-(1R,2R)-1,2-cyclohexanediylimino(1-oxo-1,2-ethanediyl)], rel- (9CI) (CA INDEX NAME)

As soluble complexan polymer in organic solvents, derived from 1,2-diaminocyclohexane-N,N,N',N'-tetraacetic acid (CyDTA), was synthesized and used as a polymer chelate precursor to YBa2Cu3O7-x thin films. Five complexan polymers (3) were prepared by a ring-opening polyaddn. of CyDTA dianhydride (1) with several diamines (2). The polymer (3e) prepared with 1,2-diaminocyclohexane (2e) was soluble in water, DMSO (DMSO), methanol, and ethanol. A clear aqueous solution (pH 8) containing 3e and 1/2 equiv molar amount of

metal nitrates of Y, Ba, and Cu (1:2:3 in molar ratio) was poured into tetrahydrofurane (THF) to precipitate a polymer-metal chelate. The chelate formations of each metal were confirmed by C=O stretching bonds. The polymer chelate precursor was soluble in methanol, DMSO, and water, and partially soluble in ethanol. The polymer-metal chelate was dissolved in

methanol, of which the metal concentration was adjusted to 3 wt%. This solution was

spin-coated onto SrTiO3 (100) and MgO (001) substrates for preparing YBa2Cu3O7-x thin films. According to an X-ray diffraction anal., YBa2Cu3O7-x film with a c-axis orientation was formed on a SrTiO3 substrate; even the precursor film was sintered at 780 °C for 1 h under air. Superconducting YBa2Cu3O7-x films with a c-axis orientation were also prepared on a MgO (001) substrate.

REFERENCE COUNT:

THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 28 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2001:114146 CAPLUS

DOCUMENT NUMBER:

134:290215

TITLE:

Effect of the long-acting tachykinin NK1 receptor antagonist MEN 11467 on tracheal mucus secretion in

allergic ferrets

AUTHOR (S):

Khan, Safina; Liu, Yu-Chih; Khawaja, Aamir M.;

Manzini, Stefano; Rogers, Duncan F.

CORPORATE SOURCE:

Thoracic Medicine, National Heart & Lung Institute,

Imperial College, London, SW3 6LY, UK

SOURCE:

British Journal of Pharmacology (2001), 132(1),

189-196

CODEN: BJPCBM; ISSN: 0007-1188

PUBLISHER:

Nature Publishing Group

DOCUMENT TYPE:

Journal English

LANGUAGE:

11467

IT 214487-46-4, MEN 11467

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(effect of tachykinin NK1 receptor antagonist MEN 11467 on tracheal mucus secretion in allergic ferrets)

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

We investigated the effect of MEN 11467 ((1R,2S)-2-N[1(H)indol-3-yl-carbonyl]-1-N- $\{N\alpha(p-tolylacetyl)-N\alpha(methyl)-D-3-(2-naphthyl)alanyl\}$ diaminocyclohexane) on tachykinin-induced mucus secretion in ferret trachea in vitro and determined its effect on secretion by tracheae from allergic ferrets in response to allergen challenge. Repeated administration of [Sar9,Met(O2)11]-substance P ([Sar9]SP, 1  $\mu$ M) maintained mucus output above control values for at least 1.75 h. MEN

11467 inhibited secretion in a concentration-dependent manner with maximal inhibition at 10  $\mu M$  and an approx. IC50 of 0.3  $\mu M$ . Inhibition by MEN 11467 (0.1-10  $\mu M$ ) was maintained, to varying degree, for at least 1.75 h after washout in the continued presence of [Sar9] SP. In elec. stimulated tracheae, tachykininergic neural secretion was virtually abolished by 1 µM MEN 11467. In tracheae from ovalbumin-sensitized animals, repeated administration of ovalbumin maintained mucus output above controls for 1.5 h. MEN 11467 inhibited ovalbumin-induced secretion in a concentration-dependent manner, with complete inhibition at 1  $\mu\text{M}\,.$ Inhibition by MEN 11467 (1 and 10  $\mu$ M) was maintained, to varying degree, after drug washout for the 1.5 h of ovalbumin stimulation. 11467 1  $\mu M$  did not affect secretion induced by either acetylcholine or histamine, whereas 10  $\mu M$  MEN 11467 did inhibit agonist-induced secretion. We conclude that, in ferret trachea in vitro, MEN 11467 at concns. of 0.1-1  $\mu M$  is a long acting and selective inhibitor of tachykininergic-induced mucus secretion, and may have therapeutic potential for bronchial hypersecretion associated with allergic conditions, for example in asthma.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 29 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:31282 CAPLUS

DOCUMENT NUMBER:

134:80813

TITLE:

Use of substance P antagonists in the treatment of

adenocarcinomas

INVENTOR(S):

Pompei, Pierluigi; Massi, Maurizio; Nabissi, Massimo;

Sparapani, Pier Luigi

PATENT ASSIGNEE(S):

Innova Limited, UK

SOURCE: PCT Int. Appl., 10 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
	A2 20010111	WO 2000-EP6309	20000705
WO 2001001922			
W: AE, AG, AL,	AM, AT, AU, AZ,	BA, BB, BG, BR, BY, BZ	, CA, CH, CN,
CR, CU, CZ,	DE, DK, DM, DZ,	EE, ES, FI, GB, GD, GE	GH, GM, HR,
		KG, KP, KR, KZ, LC, LK	
		MW, MX, MZ, NO, NZ, PL	
		TM, TR, TT, TZ, UA, UG	
		KZ, MD, RU, TJ, TM	
		SL, SZ, TZ, UG, ZW, AT	BE, CH, CY,
		IE, IT, LU, MC, NL, PT	
		ML, MR, NE, SN, TD, TG	
IT 1306165	B1 20010530	IT 1999-RM426	19990705
		CA 2000-2373960	
		AU 2000-65616	
		EP 2000-953011	
		GB, GR, IT, LI, LU, NI	
			i, 35, MC, FI,
	LV, FI, RO, MK,		00000505
		JP 2001-507420	
US 6576638	B1 20030610	US 2002-30305	20020513
PRIORITY APPLN. INFO.:		IT 1999-RM426	
		WO 2000-EP6309	W 20000705

IT 214487-46-4, MEN 11467 214487-46-4D, MEN 11467, derivs.

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(substance P antagonists in treatment of adenocarcinoma)

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

The invention discloses the use of antagonists of neurokinin receptors (NK-1; substance P receptors) to establish a new drug effective in the treatment of adenocarcinomas, the antagonists being ≥1 substances selected among those ones having the following features: pA2>6.0 both in human and in murine tissues, etherocyclic non-peptidergic structures, antiangiogenic effects exptl. demonstrated in genitourinary tract tumors induced via orthotopic grafts of human tumor cells either in the genitourinary apparatus of either immunodeficient rats or mice, decrease of tumor mass on tumors of the genitourinary tract induced by orthotopic grafts of tumor cells onto tissues of the genitourinary tract of either immunodeficient rats or mice.

L11 ANSWER 30 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:836249 CAPLUS

DOCUMENT NUMBER: 134:147352

TITLE: Amide catalysts with tetradentate ligands and the

asymmetric transfer hydrogenation of carbonyl

compounds

AUTHOR(S):

Marson, C. M.; Schwarz, I.

CORPORATE SOURCE:

Department of Chemistry, University College London, Christopher Ingold Laboratories, London, WC1H OAJ, UK

SOURCE:

Tetrahedron Letters (2000), 41(46), 8999-9003

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: DOCUMENT TYPE: Elsevier Science Ltd.

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 134:147352

IT 323187-43-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of amidic tetradentate ligands as catalysts for asym. transfer

hydrogenation of carbonyl compds.)

323187-43-5 CAPLUS RN

Carbamic acid, [(1,2-dioxo-1,2-ethanediyl)bis[imino-(1R,2R)-2,1-CN

cyclohexanediyl]]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Amidic tetradentate catalysts comprising two trans-1,2-cyclohexanediamine AΒ units linked via a dicarbonyl spacer are shown to provide useful enantiomeric excesses in the asym. transfer hydrogenation from propan-2-ol to aromatic ketones. N-benzylation of the terminal amino groups results, in several cases, in reversal of the absolute configuration of the major product.

REFERENCE COUNT:

THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 31 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

33

2000:628111 CAPLUS ACCESSION NUMBER:

133:222443 DOCUMENT NUMBER:

Regioselective synthesis of DTPA derivatives TITLE:

Chinn, Paul; Gyorkos, Albert; Labarre, Michael J.; INVENTOR (S):

Ruhl, Steve; Ryskamp, Thomas

Idec Pharmaceuticals Corporation, USA PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 48 pp.

CODEN: PIXXD2

Patent DOCUMENT TYPE: English LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

APPLICATION NO. DATE DATE PATENT NO. KIND

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                                                WO 2000-US5433
                                                                          20000302
     WO 2000051976
                            A1
                                   20000908
         W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
              CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
              SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ,
              BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
              DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
              CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                US 1999-261207
                                                                          19990303
                            B1
                                   20010327
     US 6207858
                                   20000908
                                                CA 2000-2364960
                                                                          20000302
     CA 2364960
                            AA
     EP 1157004
                            A1
                                   20011128
                                                EP 2000-913703
                                                                          20000302
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO
                                   20011226
                                                BR 2000-8693
                                                                          20000302
     BR 2000008693
                            Α
                                                                          20000302
                                   20041223
                                                AU 2000-35099
     AU 778816
                            B2
                                                ZA 2001-6750
                                                                          20010815
     ZA 2001006750
                            Α
                                   20021115
     NO 2001004194
                                   20011026
                                                NO 2001-4194
                                                                          20010829
PRIORITY APPLN. INFO.:
                                                US 1999-261207
                                                                      A 19990303
                                                                      W
                                                WO 2000-US5433
                                                                          20000302
                           CASREACT 133:222443
OTHER SOURCE(S):
     290836-17-8P
     RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
     preparation); PREP (Preparation); RACT (Reactant or reagent)
         (regioselective synthesis of DTPA derivs.)
RN
     290836-17-8 CAPLUS
     Carbamic acid, [(1S)-2-[[(1S,2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]cy
CN
     clohexyl]amino]-1-[(4-nitrophenyl)methyl]-2-oxoethyl]-, 1,1-dimethylethyl
```

Absolute stereochemistry.

ester (9CI)

(CA INDEX NAME)

The title process for synthesizing a substantially isomerically pure DTPA derivative (sic) comprises regioselective coupling a monoprotected diamine and, e.g., a compound comprising an amine moiety capable of effectively coupling the DTPA derivative to Igs (sic). Thus, 4- (O2N) C6H4CH2CH(NHCO2CMe3) CO2H was coupled with H2NCHMeCH2NHCO2CMe3 to give 71.83% 4-(O2N) C6H4CH2CH(NHCO2CMe3) CONHCH2CHMeCH2NHCO2CMe3 which was converted in 5 addnl. steps to MX-DTPA.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 32 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:92927 CAPLUS

DOCUMENT NUMBER: 133:362

TITLE: Anti-tumor activity of tachykinin NK1 receptor

antagonists on human glioma U373 MG xenograft

AUTHOR(S): Palma, C.; Bigioni, M.; Irrissuto, C.; Nardelli, F.;

Maggi, C. A.; Manzini, S.

CORPORATE SOURCE: Menarini Ricerche S.p.A., Department of Pharmacology,

Pomezia, 00040, Italy

SOURCE: British Journal of Cancer (2000), 82(2), 480-487

CODEN: BJCAAI; ISSN: 0007-0920

PUBLISHER: Churchill Livingstone

DOCUMENT TYPE: Journal LANGUAGE: English

IT 214487-46-4, MEN 11467

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(tachykinin NK1 receptor antagonists antitumor activity on human glioma)

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-

methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Astrocytes harbor functional receptors to many neurotransmitters, AB including substance P (SP), an undecapeptide belonging to the tachykinin family of peptide transmitters. SP activates malignant glial cells to induce cytokine release and proliferation, both responses being relevant for tumor progression. In tumors developed in nude mice transplanted s.c. (s.c.) to U373 MG human glioma cells, the presence of SP was observed at immunohistochem. Although the administration of exogenous SP did not significantly affect the size or development of U373 MG xenograft, a role of SP in supporting glioma progression in vivo was highlighted by the tumor growth inhibition induced by highly specific and selective human tachykinin NK1 receptor antagonists (MEN 11467 and MEN 11149). The anti-tumor activity of MEN 11467 was observed both with s.c. or i.v. treatments and was partially reverted by the concomitant administration of exogenous SP. Doxorubicin did not show any activity in controlling U373 MG growth in this in vivo model. A novel therapeutic approach to treat malignant gliomas with tachykinin NK1 receptor antagonists is suggested by these findings.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 33 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:466663 CAPLUS

DOCUMENT NUMBER: 131:194198

Correlation between binding characteristics and TITLE:

functional antagonism in human glioma cells by

tachykinin NK1 receptor antagonists

AUTHOR (S):

Palma, Carla; Nardelli, Federica; Manzini, Stefano CORPORATE SOURCE:

Department of Pharmacology, Menarini Ricerche, Rome,

00040, Italy

European Journal of Pharmacology (1999), 374(3), SOURCE:

435-443

CODEN: EJPHAZ; ISSN: 0014-2999

Elsevier Science B.V. PUBLISHER:

DOCUMENT TYPE: Journal English LANGUAGE:

IT 214487-46-4, MEN 11467

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BIOL (Biological study)

(binding characteristics and functional antagonism in human glioma

cells by tachykinin NK1 receptor antagonists)

214487-46-4 CAPLUS RN

1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-CNmethylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-

oxopropyl]amino]cyclohexyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Binding characteristics and functional antagonism exerted by two AB structurally related tachykinin NK1 receptor antagonists, MEN 11467  $((1R, 2S) - 2N[1(H) indol - 3 - yl - carbonyl] - 1 - N - \{N\alpha(p-tolylacetyl) - 1 - N\alpha(p-tolylacetyl) - N\alpha$  $N\alpha$  (methyl) -D-3-(2-naphthyl) alanyl diaminocyclohexane) and FK888 (N2-[(4R)-4-hydroxy-1-(1-methyl-1H-indol-3-yl)carbonyl-L-prolyl]-N-methyl-N-phenylmethyl-L-3-(2-naphthyl)alaninamide), were investigated in the human astrocytoma cell line U373 MG. In radioligand binding studies, conducted with [3H] substance P and intact cells at 37°C, MEN 11467 bound to tachykinin NK1 receptors in an irreversible manner with a Ki value of 1.2  $\pm$  0.5 nM while FK888 bound in competitive manner with a Ki value of 4.6  $\pm$  2.2 nM. Receptor blockade by both antagonists resulted in a powerful and complete inhibition of functional responses induced by substance P, such as accumulation of the second messenger inositol monophosphate or interleukin-6 release. However, MEN 11467 showed a greater potency for blocking functional responses than FK888 despite their similar affinity for human tachykinin NK1 receptors. Moreover, MEN 11467 was more potent in inhibiting late rather than early phases of substance P-induced inositol monophosphate accumulation and its antagonism was enhanced by drug preincubation and barely affected by removal of unbound drug from the external medium, suggesting that MEN 11467 bound in a tight manner to the receptor. Such behavior was not observed with the competitive and rapidly reversible antagonist FK888. These data indicate that the small differences in the chemical structure of MEN 11467 and FK888 determine

the

different binding characteristics at the tachykinin NK1 receptor and which are responsible for the greater potency of MEN 11467 for blocking functional responses. The Ki value obtained in binding studies may be inadequate to reveal the real potency of tachykinin NK1 receptor antagonists.

REFERENCE COUNT:

26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 34 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1999:449800 CAPLUS

DOCUMENT NUMBER:

131:252257

TITLE:

Effect of MEN 11467, a new tachykinin NK1 receptor antagonist, in acute rectocolitis induced by acetic

acid in quinea-pigs

AUTHOR (S):

Cutrufo, Corrado; Evangelista, Stefano; Cirillo, Rocco; Ciucci, Alessandra; Conte, Bruno; Lopez, Giuseppe; Manzini, Stefano; Maggi, Carlo Alberto

CORPORATE SOURCE:

Department of Pharmacology, Menarini Ricerche spa,

Rome, Italy

SOURCE:

European Journal of Pharmacology (1999), 374(2),

277-283

CODEN: EJPHAZ; ISSN: 0014-2999

PUBLISHER:

Elsevier Science B.V.

DOCUMENT TYPE:

Journal English

LANGUAGE:

IT 214487-46-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(effect of MEN 11467, a new tachykinin NK1 receptor antagonist, in acute rectocolitis induced by acetic acid in guinea-pigs)

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

The aim of this study was to evaluate the effect of MEN 11467, a new potent tachykinin NK1 receptor antagonist, in an exptl. model of acute rectocolitis induced by an enema with 7.5% acetic acid in guinea-pigs. This effect was compared to that of mesalazine (5-amino-2-hydroxybenzoic acid). The injury was quantified visually by using a macroscopic injury score and histol. by using a necrosis score. In addition, changes in myeloperoxidase activity, a marker for neutrophil infiltration, and plasma protein extravasation were evaluated. The injury caused by 7.5% acetic acid was mild, affecting the superficial layers and producing a strong

edema of the submucosa. A single administration of MEN 11467 (0.3-10 mg/kg s.c., 1 h before acetic acid) reduced the macroscopic damage and necrosis score and the increase in plasma protein extravasation induced by 7.5% acetic acid in the early acute phase of the injury (death at 2.5 h). Mesalazine (100 mg/kg p.o., 1 h before) reduced the macroscopic score but not the plasma protein extravasation. Repeated administration of MEN 11467 (1-3 mg/kg s.c., -1, +6 and +23 h after 7.5% acetic acid) reduced the macroscopic score and myeloperoxidase activity but not the plasma protein extravasation induced in the late phase of acute injury (death at 24 h). At this time mesalazine markedly reduced the macroscopic score, myeloperoxidase activity and plasma protein extravasation induced by 7.5% acetic acid. These results suggest a greater involvement of tachykinin NK1 receptors in the early phase than in the late phase of colonic inflammation in response to chemical injury.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 37 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:436043 CAPLUS

DOCUMENT NUMBER: 127:105963

TITLE: Toward the Rational Design of Superoxide Dismutase

Mimics: Mechanistic Studies for the Elucidation of Substituent Effects on the Catalytic Activity of

Macrocyclic Manganese(II) Complexes

AUTHOR(S): Riley, Dennis P.; Lennon, Patrick J.; Neumann, William

L.; Weiss, Randy H.

CORPORATE SOURCE: Monsanto Company, St. Louis, MO, 63167, USA

SOURCE: Journal of the American Chemical Society (1997),

119(28), 6522-6528

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

IT 192319-86-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(superoxide dismutase mimics - catalytic activity of macrocyclic

manganese(II) complexes)

RN 192319-86-1 CAPLUS

CN Acetamide, N,N'-1,2-cyclohexanediylbis[2-[[(4-methylphenyl)sulfonyl]amino]-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

AB Two new isomeric bis(trans-fused cyclohexano) substituted

```
1,4,7,10,13-pentaazacyclopentadecane ligands and their Mn(II) complexes,
     (I) and (II), have been synthesized, and their activity as superoxide
     dismutase (SOD) catalysts has studied. Complex I is an excellent SOD
     catalyst with a second-order rate constant at pH = 7.4 of 1.2+108 M-1
     s-1. In contrast, the isomeric complex II has virtually no detectable
     catalytic SOD activity, implying the need to understand the effect that
     the position, number, and stereochem. of substituents exert on the catalytic
     rate. The crystal structure of the complex II was determined and reveals that
     the Mn(II) ion is coordinated in a pentagonal bipyramid array of the five
     nitrogens of the macrocyclic ligand and capped by two trans-chloro
     ligands. Crystal data for MnC18H37Cl2N5 are as follows: triclinic at
     20°, space group P1--Ci2 (number 2); a = 9.746(3) Å, b = 12.631(6)
     Å, c = 11.311(5) Å; \alpha = 73.14(4)^{\circ}, \beta =
     76.39(3)°, \gamma = 79.98(3)°, V = 1287(1) Å3, and Z =
     2 (pcalc = 1.279 g/cm3; \mua Mo K\alpha = 6.23 mm-1). Mechanistic
     studies with the complex I and the pentamethyl substituted complex,
     including D2O rate studies, are reported and are consistent with the
     existence of two pathways for the rate-determining electron-transfer from
Mn(II)
     to superoxide: (1) hydrogen atom transfer from a bound water on Mn(II) to
     HO2. to yield a Mn(III) hydro intermediate and (2) the dissociative
     pathway in which superoxide anion binds to a vacant coordination site on
     Mn(II) followed by protonation/oxidation to yield a Mn(III)hydroperoxo
     species. Subsequent reduction of the intermediate Mn(III) with superoxide
     anion completes the catalytic cycle. Substituent effects on the rates and
     relative contribution of the two pathways to the overall rate of SOD
     activity is ascribed to the propensity of the ligand to fold around Mn(II)
     forming a pseudo-octahedral complex similar in geometry to the oxidized
     Mn(III) complex. Folding of the pentaaza macrocyclic ligand is confirmed
     as a relevant structural motif for this series of Mn(II) complexes by the
     x-ray structure determination of the bis(nitrate) derivative,
[Mn (C10H25N5) NO3] NO3,
     which reveals a six-coordinate structure with a folded conformation of the
     macrocyclic ligand. Crystal data for [Mn(C10H25N5)NO3]NO3: orthorhombic
     at -100°C, space group P212121; a = 9.457(2) \text{ Å}, b = 12.758(2)
     Å, C = 13.834(2) Å, V = 1669.1(5) Å3, and Z = 4 (pcalc =
     1.549 \text{ g/cm3}).
                               THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                         35
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L11 ANSWER 38 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
                         1996:612907 CAPLUS
ACCESSION NUMBER:
                         125:315168
DOCUMENT NUMBER:
                         Cobalt(III) complexes of N, N'-bis(2(S)-aminopropyl)-
TITLE:
                          1(R),2(R)-trans-1,2-diaminocyclohexane
                         Lee, Dong-Il; Jun, Moo-Jin
AUTHOR (S):
                         Dep. of Chemistry, Yonsei Univ., Seoul, 120-749, S.
CORPORATE SOURCE:
                         Korea
                         Bulletin of the Korean Chemical Society (1996), 17(9),
SOURCE:
                          786-790
                         CODEN: BKCSDE; ISSN: 0253-2964
                         Korean Chemical Society
PUBLISHER:
                         Journal
DOCUMENT TYPE:
                         English
LANGUAGE:
     183255-16-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
        (for preparation of optically active bis(aminopropyl)diaminocyclohexane and
        its cobalt complexes)
```

RN 183255-16-5 CAPLUS

CN Propanamide, N,N'-1,2-cyclohexanediylbis[2-amino-, dihydrochloride,  $[1R-[1\alpha(S^*),2\beta(S^*)]]$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} \text{Me} & \text{S} & \text{NH} \\ \text{H}_2\text{N} & \text{R} & \text{N} & \text{S} \\ \end{array}$$

#### •2 HCl

AB A novel optically active tetraamine ligand possessing four asym. centers, N,N'-bis(2(S)-aminopropyl)-1(R),2(R)-trans-1,2-diaminocyclohexane (SRRS-apchxn) and its cobalt(III) complexes, [Co(SRRS-apchxn)X2]n+ (X = Cl-, H2O; X2 = CO32-) were synthesized. This ligand has coordinated stereospecifically to the cobalt(III) ion to give only the  $\Lambda$ -uns-cis(SS) isomer. A trans dichloro complex was obtained via the stereospecific isomerization of  $\Lambda$ -uns-cis(SS)-[Co(SRRS-apchxn)Cl2]+ to trans-(SS)-[Co(SRRS-apchxn)Cl2]+ in CH3OH-HCl medium. Ligand and complexes were characterized by electronic absorption, 1H NMR, CD spectra, and also by elemental anal. It is of interest that this is one of the few CoIII(N4)X2 type complex prepns., which produces such an uns-cis isomer with stereospecificity.

L11 ANSWER 41 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1992:448054 CAPLUS

DOCUMENT NUMBER:

117:48054

TITLE:

Synthesis of C-functionalized trans-

cyclohexyldiethylenetriaminepentaacetic acids for labeling of monoclonal antibodies with the bismuth-212

 $\alpha$ -particle emitter

AUTHOR(S):

Brechbiel, Martin W.; Gansow, Otto A.

CORPORATE SOURCE:

Radiat. Oncol. Branch, Natl. Cancer Inst., Bethesda,

MD, 20892, USA

SOURCE:

Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1972-1999)

(1992), (9), 1173-8

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE:

Journal

LANGUAGE: OTHER SOURCE(S): English CASREACT 117:48054

IT 142350-86-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with hydrogen bromide)

RN 142350-86-5 CAPLUS

CN Carbamic acid, [2-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-

nitrophenyl)-1-oxopropyl]amino]cyclohexyl]-, phenylmethyl ester,  $[1R-[1\alpha,2\beta(S^*)]]-(9CI)$  (CA INDEX NAME)

Absolute stereochemistry.

Several C-functionalized cyclohexyldiethylenetriaminepentaacetic acid AB derivs. have been prepared from  $(\pm)$ -4-nitrophenylalanine and (±)-trans-cyclohexane-1,2-diamine to produce two sets of diastereoisomeric enantiomers. A modification of this synthesis has been employed to prepare a single enantiomer in order to define the absolute configurations of the products.

L11 ANSWER 42 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1992:443667 CAPLUS

DOCUMENT NUMBER:

117:43667

TITLE:

N, N' - (2-aminoethyl) -trans-1, 2-diaminocyclohexane-

N,N',N'',N''',N''''-hexaacetic acid and related compounds for chelating agents for immunoconjugates

INVENTOR(S):

Mease, Ronnie C.; Srivastava, Suresh C.; Gestin, Jean

Francois

PATENT ASSIGNEE(S):

Associated Universities, Inc., USA

SOURCE:

U.S., 13 pp. Cont.-in-part of U.S. 5,021,571.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
US 5089663	Α	19920218	US 1991-679258	19910402	
US 5021571	Α	19910604	US 1989-372905	19890629	
US 5334729	Α	19940802	US 1991-787244	19911104	
PRIORITY APPLN. INFO.:			US 1989-372905 A	2 19890629	
			US 1991-679258 A	3 19910402	

#### 137731-40-9P 137731-42-1P 137820-29-2P IT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in cyclohexyl polyaminocarboxylate derivative preparation for radiolabeled immunoconjugate preparation)

RN 137731-40-9 CAPLUS

Carbamic acid, [1,2-cyclohexanediylbis[imino(2-oxo-2,1-ethanediyl)]]bis-, CN

bis(1,1-dimethylethyl) ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 137731-42-1 CAPLUS

CN Carbamic acid, [2-[[[(1,1-dimethylethoxy)carbonyl]amino]acetyl]amino]cycl ohexyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 137820-29-2 CAPLUS

CN Acetamide, N,N'-1,2-cyclohexanediylbis[2-amino-, dihydrochloride, trans-(9CI) (CA INDEX NAME)

Relative stereochemistry.

●2 HCl

AB Rigid chelating structures are disclosed, as are their preparation and their use in preparing radiometal-labeled immunoconjugates. The compds. of the

invention include cyclohexyl EDTA monoanhydride, the trans forms of cyclohexyl DTPA and TTHA, and derivs. of these cyclohexyl polyaminocarboxylate materials. The title compound is specifically claimed. Biodistribution of radiometal-labeled immunoconjugates is included. Cyclohexyl EDTA immunoconjugates (from both monoanhydride and N-hydroxysuccinimide derivs.) with anti-colon cancer antibody 17-1A were superior to the nonrigid counterparts with respect to tumor uptake.

L11 ANSWER 46 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1981:498228 CAPLUS

DOCUMENT NUMBER:

95:98228

TITLE:

2-Deoxy-2-substituted fortimicin A and B and

derivatives

INVENTOR(S):

Johnson, Paulette; Martin, Jerry R.; Nadzan, Alex M.;

Tadanier, John S.

PATENT ASSIGNEE(S):

Abbott Laboratories, USA

SOURCE:

U.S., 13 pp. CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4250304	A	19810210	US 1979-79145	19790926
AU 8061991	A1	19810402	AU 1980-61991	19800903
GB 2059958	Α	19810429	GB 1980-29336	19800911
ES 495313	A1	19811016	ES 1980-495313	19800924
BE 885402	A1	19810325	BE 1980-202235	19800925
FR 2465743	A1	19810327	FR 1980-20601	19800925
FR 2465743	В1	19830708		
DE 3036185	A1	19810416	DE 1980-3036185	19800925
JP 56057799	A2	19810520	JP 1980-133150	19800926
PRIORITY APPLN. INFO.:			US 1979-79145	A 19790926

#### IT 78027-31-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenolysis of)

78027-31-3 CAPLUS RN

L-chiro-Inositol, 1,4,5-trideoxy-6-0-methyl-1-CN

[methyl[[[(phenylmethoxy)carbonyl]amino]acetyl]amino]-3-0-[2,3,4,6,7-

pentadeoxy-2,6-bis[[(phenylmethoxy)carbonyl]amino]-β-L-lyxoheptopyranosyl]-4-[[(phenylmethoxy)carbonyl]amino]-5-

[[[[(phenylmethoxy)carbonyl]amino]acetyl]amino] - (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

GI

AB Fortimicins I (R = H, glycyl,  $\beta$ -alanyl, Ac,  $\beta$ -aminoalkyl; R1 = H, NH2, N3, halo, glycylamido,  $\beta$ -alanylamido, 2-O-methanesulfonyl; R2 = H, halo; R1 = R2  $\neq$  H), with antibacterial activity, were prepared Thus, fortimicin B in 4 steps was converted into 1,2',6'-tri-N-benzyloxycarbonyl-2-O-methanesulfonylfortimicin B, which was treated with N-hydroxysuccinimide ester of N-benzyloxycarbonylglycine and the product hydrogenolyzed over Pd/C to give 2-O-methanesulfonylfortimicin A.4HCl

(II). A solution of II was passed through a column of anion exchange resin, basic eluate was allowed to stand at room temperature for 120 h, the solution was

concentrated and again was passed through an anion exchange resin column to give

2-deoxy-1,2-epiminofortimicin A, which was treated with NaN3 to give I.4HCl (R = H2NCH2CO, R1 = N3, R2 = H) (III). Min. inhibitory concentration of III against Staphylococcus aureus Smith is 3.1 µg/mL.

L11 ANSWER 47 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1974:485380 CAPLUS

DOCUMENT NUMBER:

81:85380

TITLE:

Stereochemical studies of N-methyl-(S)-

alaninatocobalt(III) complexes with chiral tetramines.

II. Cobalt(III)-N-methyl-(S)- and

(R)-alaninate-N, N'-bis ( $\beta$ -aminoethyl)-1(R),

2(R)-diaminocyclohexane systems Saburi, Masahiko; Yoshikawa, Sadao

AUTHOR(S): CORPORATE SOURCE:

Fac. Eng., Univ. Tokyo, Tokyo, Japan

SOURCE:

Bulletin of the Chemical Society of Japan (1974),

47(5), 1184-9

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE:

Journal

LANGUAGE:

English

TΤ 53719-90-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) 53719-90-7 CAPLUS

RN Acetamide, N,N'-1,2-cyclohexanediylbis[2-amino-, dihydrochloride, CN

(1R-trans) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### ●2 HCl

AB

For diagram(s), see printed CA Issue. GI

The preparation and structural assignments of N-methyl-(S)- and

-(R)-alaninato-cobalt(III) complexes with N,N'-bis( $\beta$ -aminoethyl)-

1(R),-2(R)-diaminocyclohexane[(R)-baetchxn] are described. The

 $\Lambda$ - $\beta$ 2(SSR) isomer I was obtained for Co(N-Me-(S)-Ala)

[(R)-baetchxn]2+ ion. The two isomers, which were found for the

Co-[N-Me-(R)-Ala] [(R)-baetchnx]2+ ion under equilibrium condition at pH 7, are assigned as the  $\Lambda$ - $\beta$ 2(SSR) and  $\Lambda$ - $\beta$ 2(SSS)

configurations, taking into account the stereospecific coordination of the

(R)-baetchxn. The stereoisomerism of  $\Delta$ - $\beta$ 2-Co(N-Me-(S)-Ala)

(trien)2+ ion is also discussed. The structures of 2 species observed in the

PMR measurements of Co(N-Me-(R)-Ala) ((R)-baet-chxn)2+ ion and assigned to  $\Lambda$ - $\beta$ 2(SSR) II and  $\Lambda$ - $\beta$ 2(SSS) III configurations, resp., are determined, based on the chemical shifts of  $\alpha$ -methine protons of N-methylalaninate moieties.

L11 ANSWER 49 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1969:501371 CAPLUS

DOCUMENT NUMBER: 71:101371

TITLE: Synthesis of a new triethylenetetramine homolog

containing four optically pure centers. Some stereoselective cobalt(III) ion complexes of this

ligand

AUTHOR(S): Asperger, Robert G.

CORPORATE SOURCE: Biochem. Res. Lab., Dow Chem. Co., Midland, MI, USA

SOURCE: Inorganic Chemistry (1969), 8(10), 2127-31

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 24125-68-6P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 24125-68-6 CAPLUS

CN Hydrocinnamamide, N,N'-1,2-cyclohexylenebis  $[\alpha-amino-,$ 

dihydrochloride (8CI) (CA INDEX NAME)

# ●2 HCl

GI For diagram(s), see printed CA Issue.

AB The synthesis of a new tetramine ligand, N,N'-bis(L-2-amino-3-phenylpropyl)-trans-D-1,2-cyclohexanediamine (I), a homolog of triethylene-tetramine which contains four optical centers, is reported. The syntheses of the L-cis- $\beta$ - and optically active trans-cobalt(III) perchlorate derivs. are reported. Absorption and O.R.D. spectra are reported and used, along with some chemical data, to assign the configurations of the isomer.

L11 ANSWER 50 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1969:73647 CAPLUS

DOCUMENT NUMBER: 70:73647

TITLE: Stereochemical studies of metal chelates. III.

Preparation and stereochemistry of cobalt(III)

complexes with C-substituted triethylenetetramines at

the central ethylenediamine bridge

AUTHOR(S): Goto, Masafumi; Saburi, Masahiko; Yoshikawa, Sadao

CORPORATE SOURCE: Univ. Tokyo, Tokyo, Japan

SOURCE:

IT

Inorganic Chemistry (1969), 8(2), 358-66

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE:

Journal English

LANGUAGE:

22559-12-2P 22559-13-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 22559-12-2 CAPLUS

CN Carbamic acid, [1,2-cyclohexylenebis(iminocarbonylmethylene)]di-, dibenzyl

ester, trans- (8CI) (CA INDEX NAME)

Relative stereochemistry.

RN 22559-13-3 CAPLUS

CN Carbamic acid, [1,2-cyclohexanediylbis[imino(2-oxo-2,1-ethanediyl)]]bis-, bis(phenylmethyl) ester, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

The preparation of dichloro- and dinitrocobalt(III) complexes of optically active C-substituted triethylenetetramine at the central ethylenediamine bridge is described. The stereoselective formation of the cis- $\beta$  isomer was observed and the stereochem. details are discussed in terms of the conformation of each chelate ring as well as the configurations of the secondary N atoms. The rearrangement of cis- $\beta$ -dichloro complexes to trans-isomers is also reported.

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